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Conversion of Omega-3 Fatty Acids from Algae Biomass Produced Biodiesel

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Abstract
As the effects of global warming continue to escalate, carbon-neutral fuels are becoming sought after alternatives to traditional fossil fuels. Biodiesel is a promising source of carbon-neutral fuel that can be produced from organisms such as algae. A new process has been proposed by Yadav for algal oil extraction using sonic waves and carbon dioxide microbubbles (Yadav et al., 2019). Although a novel idea, it currently struggles to compete economically with other types of biodiesel production as well as traditional food sources. However, a small subsection of the FAMEs is able to be further processed into Omega-3 fatty acids. These fatty acids can be added to foods as nutraceutical supplements and can be sold for a higher price than biodiesel. This proposal attempts to modify a theoretical algae-to-biodiesel process to separate these valuable FAMEs from the other biodiesel products and produce approximately 12,000 tons/yr of raw Omega-3 supplement. The process utilizes liquid-liquid extraction to remove the methyl EPA and methyl DHA from the biodiesel and then uses base-catalyzed ester hydrolysis to convert the long chain methyl esters into their marketable carboxylic acid form. The proposed plant will produce 547,830 US-tons of biodiesel which satisfies 10% of the current biodiesel market, 12,000 US-tons of Omega-3 fatty acids, and 39,683 US-tons of crude glycerol per year. This production level 30% of the United States Omega-3 market in 2024, and 6% of the current glycerol market. A financial analysis of manufacturing the plant to separate desired FAMEs and hydrolyze them to the Omega-3s over a 20-year period shows that this process could be profitable to a varying degree based on the sale price of the Omega-3s. The profitability of this design is contingent on a few factors, such as being able to access the right markets to sell the raw Omega-3 product being formed and how the market for these supplements will grow in the future. Thus, this proposal can recommend, with some hesitation, pursuing the modifications to the plant to co-produce biodiesel with Omega-3 fatty acids.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

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School of Engineering and Applied Science
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220 S. 33rd Street Philadelphia, PA 19104
April 23, 2019

Dear Dr. Warren D. Seider and Mr. Bruce M. Vrana,

Enclosed is a potential process design for the separation of Omega-3s fatty acids from fatty acid methyl esters (FAMEs) produced from algae and their conversion to a marketable form. This design builds on the work of Geetanjali Yadav, Leonard Fabiano, and Dr. Warren Seider to produce algae-based biodiesel and explores whether making the Omega-3 fatty acids can make the biodiesel design profitable. The enclosed process can produce 547,830 US-tons of biodiesel, 12,000 US-tons of Omega-3 fatty acids, and 39,683 US-tons of crude glycerol per year. This production level satisfies 10% of the current biodiesel market, 30% of the United States Omega-3 market in 2024, and 6% of the current glycerol market. The biodiesel is the main product of the plant and meets industrial biodiesel purity standards. The process employs measures to recycle all raw materials and catalysts used, properly treat waste products, and have an overall safe working environment when possible.

The plant will operate for 24 hours a day, 330 days a year. Because reducing the sales price was the primary goal of this report, rigorous profitability analysis was performed on many potential scenarios varying the purchase price and sales price of the FAMEs raw material and biodiesel and Omega-3 sales prices. The total capital investment of the plant is $12.1MM. Several scenarios were identified at which the plant would be profitable with at least an IRR of 15%. We recommend moving forward in developing the proposed process enclosed, but emphasize that additional research into the areas of market pricing, FAMEs separation at industrial scale and solubility of long chain fatty acids are essential to confirm the viability of the proposed process design at industrial scale.

Sincerely,

Jacquelyn Stokes | Ryan Tu | Matthew Peters

Conversion of Omega-3 Fatty Acids from Algae Biomass Produced Biodiesel

Matthew Peters
Jacquelyn Stokes
Ryan Tu

Proposed by: Dr. Warren Seider, Dr. Leonard Fabiano, Geetanjali Yadav
Project Advisor: Dr. Warren Seider

University of Pennsylvania
School of Engineering
Department of Chemical and Biomolecular Engineering

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Glossary

Abbreviation	Word
ASTM	American Society for Testing and Materials
DHA	Docosahexaenoic Acid
EPA	Eicosapentaenoic Acid
FAME(s)	Fatty Acid Methyl Ester(s)
GOED	Global Organization for EPA/DHA Omega-3
HCl	Hydrochloric Acid
HTL	Hydrothermal Liquefaction
IRR	Investors Rate of Return
LLE	Liquid-Liquid Extraction
NaOH	Sodium Hydroxide
NPV	Net Present Value
PNNL	Pacific Northwest National Laboratory
ROI	Return on Investment

1. Abstract

As the effects of global warming continue to escalate, carbon-neutral fuels are becoming sought after alternatives to traditional fossil fuels. Biodiesel is a promising source of carbon-neutral fuel that can be produced from organisms such as algae. A new process has been proposed by Yadav for algal oil extraction using sonic waves and carbon dioxide microbubbles (Yadav et al., 2019). Although a novel idea, it currently struggles to compete economically with other types of biodiesel production as well as traditional food sources. However, a small subsection of the FAMEs is able to be further processed into Omega-3 fatty acids. These fatty acids can be added to foods as nutraceutical supplements and can be sold for a higher price than biodiesel. This proposal attempts to modify a theoretical algae-to-biodiesel process to separate these valuable FAMEs from the other biodiesel products and produce approximately 12,000 tons/yr of raw Omega-3 supplement. The process utilizes liquid-liquid extraction to remove the methyl EPA and methyl DHA from the biodiesel and then uses base-catalyzed ester hydrolysis to convert the long chain methyl esters into their marketable carboxylic acid form. The proposed plant will produce 547,830 US-tons of biodiesel which satisfies 10% of the current biodiesel market, 12,000 US-tons of Omega-3 fatty acids, and 39,683 US-tons of crude glycerol per year. This production level 30% of the United States Omega-3 market in 2024, and 6% of the current glycerol market. A financial analysis of manufacturing the plant to separate desired FAMEs and hydrolyze them to the Omega-3s over a 20-year period shows that this process could be profitable to a varying degree based on the sale price of the Omega-3s. The profitability of this design is contingent on a few factors, such as being able to access the right markets to sell the raw Omega-3 product being formed and how the market for these supplements will grow in the future. Thus, this proposal can recommend, with some hesitation, pursuing the modifications to the plant to co-produce biodiesel with Omega-3 fatty acids.

2. Introduction and Objective Time Chart

2.1 Background

With a population currently at 7.6 billion and quickly growing, the increasing human population combined with ever exponentially increasing technology has caused the energy requirements for the world to become larger and larger every day. In 1995, global usage of energy was estimated by the US Energy Information Administration (EIA) to be 386 EJ or 386 times ten to the eighteen joules. Twenty years later, in 2015, that number nearly doubled as energy usage reached 607EJ. The energy usage of the world is expected to continue to rise. The EIA has extrapolated that in 2035 the world's energy usage will reach 728 EJ (EIA, 2018). With an ever-growing need for energy, it is essential to consider how this energy is produced and what consequences it has on humans, the environment, and global warming.

Eighty-three percent of the world's energy is made up of oil, natural gas, and coal, sources that when used, have significant repercussions for the earth's environment as well as human health. Many believe we need alternative energy sources because we are running out of traditional types of fuel. However, with recent improvements in drilling technology like fracking, traditional fuels are still readily available. According to BPs international statistics, there are enough product reserves of coal, gas, and oil to fuel the world under current economic and operating conditions for 113, 53, and 51 years respectively (BP, 2019). Therefore, there is no shortage of traditional fuels for the world to use. However, there are other reasons why using traditional fuels for over 75% of the world's energy is a bad idea. Coal, gas, and oil have several environmental and social impacts including air pollution, oil spills, methane leakages, explosions, acid rain, and land loss. However, the largest issue with conventional fuel sources is their effect on greenhouse gas levels that cause global temperature and climate change.

The economic and population growth in the past century and a half has led to unprecedented amounts of carbon dioxide, methane, and nitrous oxide in the atmosphere. The implications of the continual increase of carbon dioxide and other greenhouse gases in the atmosphere are global warming, sea level rises, and the destruction of the ozone layer in the earth's atmosphere which protects us from harmful solar radiation. Therefore, it is essential that we explore alternatives to traditional fuel sources that flood our atmosphere with greenhouse gases.

2.1.1 Carbon-Neutral Fuel Sources

Promising alternatives to the traditional fossil fuels are “carbon-neutral” technologies. Biodiesel is especially promising as it is derived from renewable resources like plants that also absorb solar radiation. This fuel can help provide the United States a source of renewable energy that is carbon-neutral but still easily used as it is in a form similar to fossil fuels. Biofuel can be produced from many different feedstocks including first generation like corn, or second-generation like waste products and used cooking oil. Although both of these types of feedstock are effective ways to produce biodiesel, both are hard to produce on a large scale because of limitations on the source feedstock: corn is also sold as food, and there are not enough waste products to use with the current technology.

The most promising feedstocks for biofuel production are third generation feedstocks. These are feedstocks grown explicitly to produce biodiesel. Species like Miscanthus genus and microalgae can grow well in locations unsuitable for food crops and have lipid compositions. Microalgae is even more promising as it can grow and prosper in many conditions at varying temperatures, levels of light, and in either fresh or salt water depending on the species. Algae, therefore, is a highly promising feedstock to produce biodiesel. Biodiesel struggles to compete with the broader fuel market because it is generally more expensive to grow and produce than traditional fuel sources, especially with the improvement of fracking technology in the United States. Therefore, a significant amount of research is currently being conducted into new methods to increase the growth and productivity of algae and to improve the oil separation process to produce biodiesel. This senior design project aims to assist in creating an economically viable process for the sale of biodiesel at a competitive price to other production methods of biodiesel as well as traditional fossil fuels.

2.1.2 Proposed Algae Process

Through a series of ongoing research projects at the University of Pennsylvania, a new method to produce biodiesel has been proposed. Doctoral student Geetanjali Yadav as well as Professors Leonard A. Fabiano, Dr. Warren D. Seider, and others at Lafayette University and Yale University have created a new process for the breakdown of algae into oil using sonic

waves and supercritical carbon dioxide (Yadav et al., 2019). The proposed project, outlined in Figure 2.1, takes algae from growth raceways, concentrates the material by adding a flocculating agent, and flows it into a cylindrical transesterification extractor. The extractor has 20,000 microbubbles of carbon dioxide circulated through its central chamber per second. The central chamber is then bombarded with sonic waves which cause the microbubbles to expand and contract in size. The changing shape and size of the bubbles combined with the sonic frequencies cause the cell walls of the algae to break apart. Breaking the cell walls releases the oils within the cells. The vessel is built such that the continuous flow into the vessel causes the product to overflow into the annular region of the cylinder. The now separated oil and biomass in water are allowed to settle in the annular region. Because of large density differences, the biomass will settle to the bottom of the region while the oil will settle at the top of the annular region. The water remaining in the middle of the region is removed and recycled to the algae raceways; the oil is skimmed off the top of the column and sent to a reactor to be converted into biodiesel.

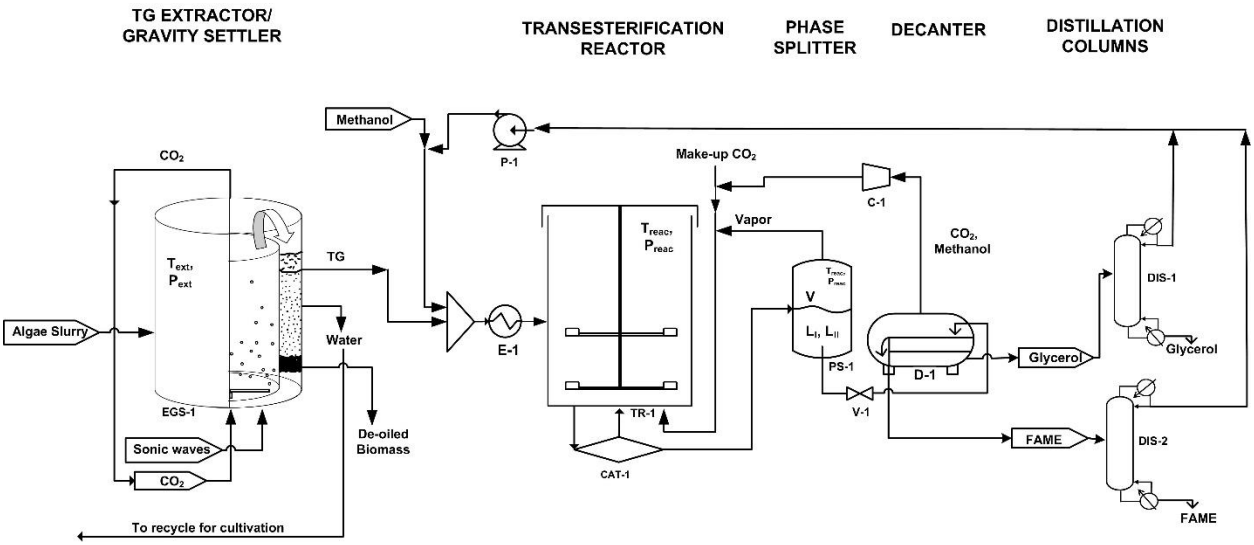


Figure 2.1 Proposed Algae Separation Process The process above has been proposed by the University of Pennsylvania team. The vessel uses carbon dioxide microbubbles and sonic waves to break apart the algae. The oil is collected through settling.

Oil from algae is converted to biodiesel through transesterification. Oil is comprised of triglycerides which are made of a glycerol backbone and three fatty acid chains of varying length. By adding excess methanol and a catalyst and reacting the mixture at 90°C and 50 bar, the triglycerides are broken apart into glycerol and fatty acid methyl esters (FAMEs). These FAMEs are highly stable derivatives of the free fatty acid chains and are how biodiesel is sold in

the United States. Following the products exit from the transesterification reactor, the products must be separated from methanol and then purified before they can be sold. This process is able to produce biodiesel at $4.34 per gallon or less (Silva et al., 2014). Although a decently competitive price, the goal of this project is to reduce the price of this process even further. This may be possible by selling the byproducts of the algae to biodiesel process: Omega-3 fatty acids.

2.1.3 Omega-3 Fatty Acids

Eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) are two types of fatty acids, which are generally long and linear carboxylic acids. In general, fatty acids range around 6 to 28 carbons long. The length is dependent on the organism which synthesizes them and the conditions in which that organism grows. The biodiesel process suggested in this study focuses on *Nannochloropsis salina,* an algal species which primarily produces fatty acid chains between 14 and 22 carbons in length. EPA, which has 20 carbons and five double bonds, and DHA, which has 22 carbons and six double bonds, can be further categorized into Omega-3 fatty acids: a categorization to describe fatty acids which have a double bond three carbons away from the terminal methyl group.

Some medical studies have shown that Omega-3s have many significant benefits to the human body (Swanson et al., 2012). EPA and DHA have been shown to reduce cardiovascular problems, assist in infant development, reduce high blood pressure, as well as act as an anti-inflammatory. These are just a few of the benefits that scientists believe a steady diet of Omega-3s can give the human body. Because of their many benefits, Omega-3s have quickly become a high demand product in the pharma and nutraceutical industry. The daily recommended dose of Omega-3s can be met from diet alone from fish, nuts, and seeds. However, many people are turning towards supplements to ensure that they get a large enough dose of Omega-3s. Today, Omega-3s are sold as separate supplement pills, prescribed as medication, and frequently put into enriched baby formulas for better child development. The Omega-3 market is continuously growing as society becomes more and more health conscious and aware of the Omega-3 fatty acids many benefits. Traditionally Omega-3 supplements are made from fish oil. Not only do these pills have an unappetizing smell and taste, but they also are not vegetarian which poses a moral dilemma for many consumers. As mentioned previously, algae also contain Omega-3s that are vegetarian and do not have an unsavory fish odor. Therefore, algal Omega-3 fatty acids are a

potentially massive money-making endeavor as an improved source of Omega-3s for supplements and pharmacology.

2.2 Motivations and Goals

As discussed in the background, the goal of this project is to make the Yadav method for producing biodiesel competitive with other types of biodiesel production as well as traditional fuels. The motivation for using this method of biodiesel production is that it requires little energy and utilizes every piece of the algae. Unlike other products, the methods proposed here save the valuable byproducts of the reaction while still keeping the whole system carbon-neutral. The goals of this project are to determine the available market and sales prices for the valuable byproducts produced. In addition, a process was designed in the hopes that it would be an economically viable way to separate the Omega-3s from the system and sell them to reduce the overall cost of the process. Finally, the main goal was to determine numerically how much the available Omega-3 sales could reduce the cost of the process per kg of biodiesel sold. This number will allow us to make an assessment to whether or not it is feasible or worthwhile to build a biodiesel facility capable of separating and producing Omega-3s.

2.3 Objective Time Chart

Name of Project: Conversion of Omega-3 Fatty Acid from Algae Biomass Produced Biodiesel

Project Leaders: Matthew Peters, Jacquelyn Stokes, Ryan Tu

Project Author: Geetanjali Yadav, Dr. Warren Seider, Mr. Leonard Fabiano

Project Advisors: Dr. Warren Seider and Bruce Vrana

Specific Goals:

- Modify a proposed algae-based biodiesel plant capable of producing 68,000 kg/hr of fatty acid methyl esters also to produce EPA and DHA
- Identify if the revenue associated with designing a plant to produce and sell EPA and DHA is enough to offset the revenue loss associated with producing biodiesel in-line with Yadav's process (Yadav et al., 2019).

Project Scope:

In Scope:

- Produce a quantity of EPA and DHA equivalent to 30% of the predicted EPA/DHA market in 2024
- Design a process starting from the flows leaving a transesterification reactor where the algae triglycerides are converted to methyl esters to isolate biodiesel
- Separate the relevant, highly unsaturated Omega-3 methyl esters from other methyl esters
- Calculate the size and cost of the equipment required for this process
- Determine if producing EPA and DHA is a viable option for making the proposed Yadav biodiesel production process profitable over a 20 year period

Out of Scope:

- Determining the quantities of algae and resources needed to produce the quantity of triglycerides being processed
- Design of process necessary to process cultivated algae to obtain triglycerides and process triglycerides to form fatty acid methyl esters
- Design of process for removal of catalyst and carbon dioxide from transesterification reactor products
- Identifying specific entities to fabricate equipment and specific locations to source materials

Deliverables:

- Process flowsheet
- Equipment design and cost
- Profitability analysis of project
- Written report and oral presentation to summarize project's conclusions

3. Innovation Map

N/A

4. Market and Competitive Analyses

The main goal of this project is to create a biodiesel process that would be competitive economically with both other renewable energy fuels but also standard fuel methods including fracking and natural gas. One of the main possible competitors to the biodiesel production process laid out in this paper is the Department of Energy Pacific Northwest National Laboratory's Hydrothermal Liquefaction Process. By using a hydrotreating reactor at a very high temperature and pressure, the Hydrothermal Liquefaction method can produce aviation grade fuel for low costs. It has been estimated that they may be able to produce biodiesel to sell for as low as $2.80 per gallon. Although an excellent sales price, because the method runs at such high temperatures and pressures, all potentially lucrative byproducts decompose during the process (DOE, 2012). Therefore, this design project aims to answer whether the sale of the byproducts can offset the price of this process design sufficiently to be competitive or more economically efficient than the PNNL's process.

As mentioned in the background, this project focuses on optimizing Yadav's process that uses carbon dioxide microbubbles and sonic waves to produce the biodiesel (Yadav et al., 2019). It has been estimated that this process could produce biodiesel at a sales price of $4.34 per gallon (Silva et al., 2014). This price is significantly higher than the cost of fossil fuels and other clean alternatives. Therefore, in order to make the production of biodiesel using this method feasible on a larger national or global scale, this price must be lowered. Our project aims to do this by selling the byproducts: primarily glycerol and the EPA/DHA Omega-3.

Glycerol is a renewable, clean-burning fuel used in many processes that are often a byproduct of the biodiesel process. Glycerol is used in many common fields including the food and pharmaceutical industries, as well as in antifreeze. It is also an important intermediate chemical for the production of nitroglycerin, propylene glycol, and epichlorohydrin: an important material used for epoxy resins. Due to its versatile use and applications across renewable energy, glycerol has been steadily increasing in popularity for the past several years as there has been a stronger push towards clean energy. Market reports indicate that glycerol production and purchasing will continue to increase for the next several years.

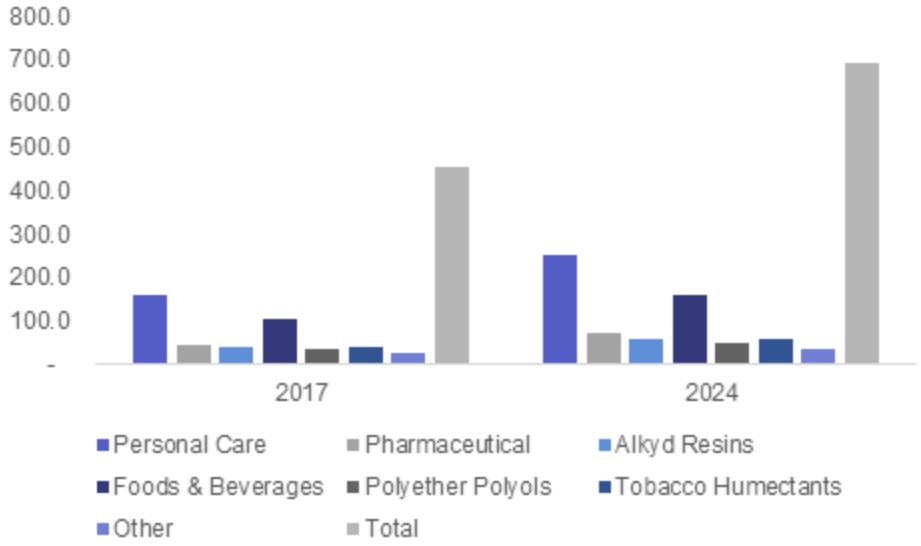


Figure 4.1. U.S. Glycerol Market Size, By Application, 2017 & 2024, (Kilo Tons)

Figure 4.1 shows the market for glycerol in 2017, divided by industry as well as a projection for 2024 when the plant would presumably be in operation. The market data suggests that by the year 2024 the demand for glycerol per year will reach approximately one million kilotons (Grand View Research, 2019). This demand bodes well for the glycerol industry as well as this process' place in it. Our estimates indicate that the glycerol produced as a byproduct in the proposed plant would be approximately 6% of the market in 2024. This amount would be a comfortable level of production that would ensure the plant would not flood the market with glycerol, but could also meet a steady demand for the product. Based on current literature and market studies, it was estimated that the 99.5% purity glycerol that the proposed plant would produce could be sold for at least $1.07/kg (Science Direct).

In addition to glycerol, the primary source of income from selling the byproducts would be from the sale of the EPA and DHA. The market for fish oil products and other Omega-3 related supplements has also been steadily increasing for the past several years. Many nutraceutical companies use EPA/DHA in their production of various medicines, supplements, infant formulas, and other consumer products. Figure 4.2 shows some of the uses of these long chain fatty acids and the expected growth of the industry until 2025 (GOED, 2014).

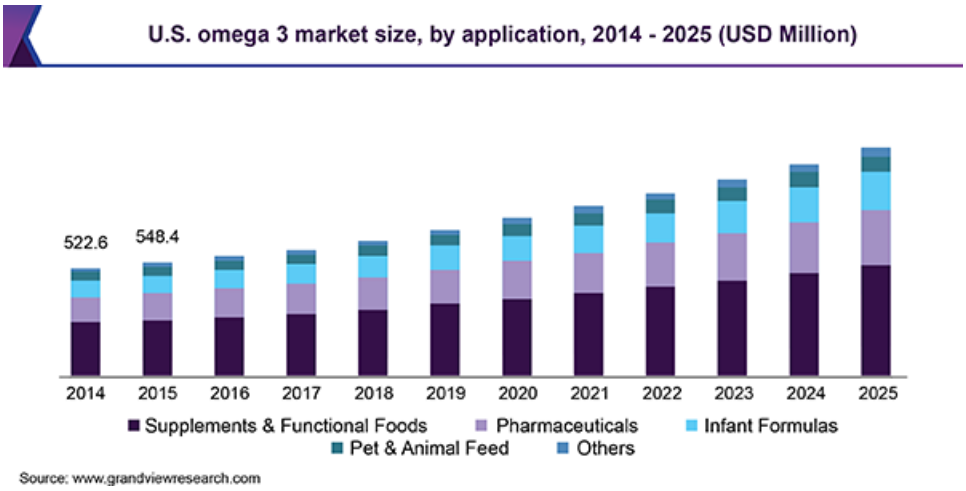


Figure 4.2. Omega-3 Market Size, 2014-2025 (predicted)

If all of the Omega-3s available in the biodiesel produced from our plant were separated and sold to the pharmaceutical industry, our proposed plant could produce nearly 100% of the current American market for Omega-3s. This amount would obviously flood the market and be completely unfeasible. Therefore, it was decided to design the plant such that enough Omega-3s would be produced per hour to match approximately 30% of the US market for EPA and DHA in 2024. While still an aggressive percentage of the market, since the industry is growing so quickly, we expect that we can comfortably sell this amount of Omega-3s without flooding the market or having large excesses of Omega-3s produced.

Additionally, the global market for Omega-3 is quite large beyond the United States, as seen in Figure 4.3 (Grand View Research, 2018).

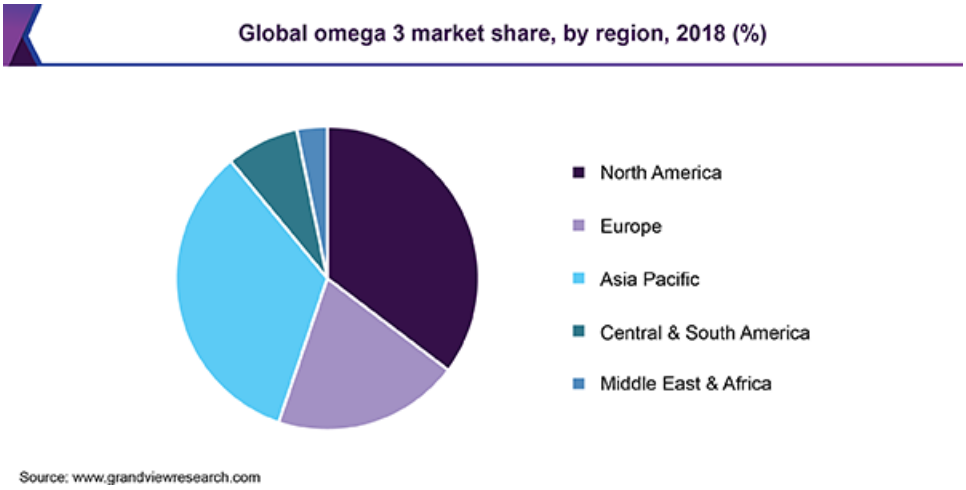


Figure 4.3 Global Market for Omega-3

When selling the EPA/DHA, close attention should be paid to potential markets in Asia and Europe, as they could provide significant sources of income. However, the cost of transportation of the production across long distances must be determined as it could outweigh the additional opportunities.

Finally, Omega-3 fatty acid can come from many different sources, primarily fish oils. However, our product would be sourced entirely from the algae and could be marketed to the more niche-vegetarian market at a premium price. It is important to note that exact quantitative data on Omega-3s sales and pricing was unavailable. Therefore, this data has pulled from bulk sale prices and other research currently available on the internet (Jedwards International Inc, 2019). However, to account for the wide range of prices found, as well as the fact that our proposed product is high purity vegetarian EPA/DHA that does not contain other oils, a wide range of prices were considered to determine the profitability of the plant. Later sections will discuss how varying the price of the Omega-3 within an expected range can drastically change the success of the plant. For this project, it was estimated that the sale of bulk Omega-3 oils could be anywhere between $15 and $120 per kg. These numbers were determined based off of bulk sale prices of fish oil found on the internet as well as the sale price of fish oil pills, taking into account at least 100% return on the retail sale (Wholmega, 2019).

5. Customer Requirements

Although FAMEs are the main products of our process, it is still important to consider the customer requirements for the byproducts that we plan to sell in the proposed process. In order to sell the glycerol and EPA and DHA that will be produced in our plant, it is essential that the product streams follow the industry's requirements for purity as well as limits on substances in oils. The first of our byproducts, crude glycerol, is an important chemical in the production of resins and gums used in protective coatings for various house paints and automotive enamels. Organizations like the ASTM have not published regulations for glycerol. However, the industry standard is that any glycerol must have a purity of at least 99.5% glycerol by weight to be considered high purity (Ahuja, 2018). This setpoint was taken into account when the proposed plant was designed such that all of the glycerol entering our process will be at least 99.5% pure. Although most industries are happy with 99.5% purity, some pharmaceutical purposes require more highly purified glycerol. However, because glycerol will not be the main source of byproduct revenue and 99.99% purity required a full vacuum distillation column, the proposed plant will sell glycerol only at 99.5% purity. This purity will not sell for as much; however, it significantly reduces the equipment and energy requirements of the proposed plant.

EPA and DHA in the carboxylic acid form are highly sought after pharmaceutical and nutritional supplements. Because of their high cost and demand, the Omega-3s will be the largest source of income from byproducts for the biodiesel plant. Therefore, it is especially important that the industry standards for EPA and DHA of pharmaceutical grade are met in the production process. Depending on the source of Omega-3s, the ratio of EPA to DHA can vary widely. Based on the current products available commercially, standard products generally have a ratio between 8 and 15 parts EPA to 1-part DHA by weight. Based on using the *N. Salina* species of microalgae, the EPA-DHA blend produced by the proposed plant has a ratio of 14.6 to 1. This lands in the higher range of available products, which is fortuitous as EPA rich products tend to sell at a higher price than more DHA heavy solutions (Grand View Research, 2019).

Because of the recent growth in the nutraceutical industry, specifically the growth of the Omega-3 market, several organizations have been created for the research, sale, and marketing of Omega-3 rich products. One of these organizations, the Global Organization for EPA and DHA Omega-3 (GOED) was established in 2006 as a nonprofit organization whose aims are to regulate the production and quality standards in the industry as well as create relationships

between purchasers and suppliers in the industry. Each year the GOED releases a voluntary monograph that sets the standards for EPA and DHA in the industry to ensure safe and high-quality products are delivered to consumers. The GOED annual monograph describes the purity requirements for EPA/DHA, gives analytical methods for determining exact concentrations, and sets standards for both high purity Omega-3s for pharmacopeial sources as well as lower purity alternatives. However, since the large majority of demand for Omega-3s lies in the nutraceutical and pharmaceutical fields, it is imperative that the proposed process produces high purity EPA and DHA, as it can be sold at significantly higher prices and in much larger quantities.

Most of the strict regulations on the purity of EPA/DHA concern the presence of environmental contaminants and heavy metals. The maximum allowed concentration of polychlorinated biphenyls (PCBs) is 0.09 mg/kg. According to the World Health Organization (WHO), the maximum concentration of dioxin-like PCBs is 3 pg/g. In terms of heavy metals, the concentration of lead (Pb) must be less than 0.05 mg/kg, less than 0.1 mg/kg for Cadmium (Cd), 0.1 mg/kg for Mercury (Hg), and 0.1 mg/kg for inorganic Arsenic (As). These regulations are set to ensure the safety of consumers who will be ingesting the final product. Since the Omega-3s produced from this process will be taken directly from source algae and converted directly into FAMEs and then their carboxylic acid form, there is little to no chance for contamination to occur. The main possibilities for contamination would include 1-hexene, methanol, and potentially more saturated fatty acids. However, the process has been optimized to reduce these contaminants. If the plant were to be built, it would be essential for quality standards that the product's composition be tested regularly to ensure no contamination.

Another important consideration for the proposed plant is how EPA and DHA will be stored. When in carboxylic acid form, Omega-3 products are highly prone to oxidation, which could cause the oil to become rancid and unusable. Therefore, to prevent oxidation, all of the equipment used after the Omega-3s have been converted to their carboxylic acid form will be padded with nitrogen. Because nitrogen is an inert gas, it will displace the oxygen and ensure no side reactions occur in the vessels. The industry standard for checking oxidations levels is by setting the maximum peroxide value for EPA and DHA to 5 meq/kg (GOED, 2019). Once again, if the plant were built, this contaminant would also be tested regularly.

While not a sellable product, the proposed process will also produce wastewater with a high salt concentration and some organic compounds. The salinity is attributed to the formation

of sodium chloride as part of the process and exceeds 3.5 g salt/L, which is the average salinity of salt water (USGS). Proper disposal of this wastewater will require either costly desalination or a dilution. This wastewater will also contain small amounts of methanol and 1-hexene, which may need to be treated. The solution to both of these concerns is to send the stream to a wastewater plant and attach a price to the cost of water treatment in determining this profitability of this process. This approach effectively places the burden of identifying a proper sink for the waste and the details of reducing these contaminant concentrations within the waste stream out of the scope of this project.

6. Critical-to-Quality Variables

N/A

7. Product Concepts

N/A

8. Superior Product Concepts

N/A

9. Competitive Analysis

N/A

10. Preliminary Process Synthesis

The main goal of this project is to economically optimize the production of biodiesel from algae using Yadav's suggested process of carbon dioxide microbubbles and sonic waves (Yadav et al., 2019). This optimization will be done by the separation and sale of high demand, high price byproducts of the process. The two main products that have potential economically are glycerol and combined methyl EPA and methyl DHA. Currently, in this process, the EPA and DHA are left in their methyl ester form and sold with the other FAMEs as biodiesel. Because EPA and DHA in the carboxylic acid form can be sold at such a high price on the pharmaceutical market, this project aims to create a plant that could produce both FAMEs and EPA and DHA to reduce the overall cost of production. The main steps of the process were identified as the purification of glycerol and FAMEs from the reactor, separation of methyl EPA/DHA from the other lighter FAMEs, and the reactions necessary to convert methyl EPA/DHA into their carboxylic acid form.

Because the suggested design in this report is only a portion of a larger process design, several assumptions had to be made to model only the second half of the overall process. The portion of the process being refined in this project begins at the feed to a decanter separating the products of the triglyceride transesterification reactor. Although the reactor had already been modeled, we still used many of Yadav's assumptions to start the process. The flow of FAMEs, as well as methanol and glycerol out of the reactor, were taken as given for this report. Also, there is a large amount of carbon dioxide in the transesterification reactor. Although the larger process does not currently remove all of the carbon dioxide before the first step in our process, we assumed that all of the carbon dioxide has already been removed from the reactor product stream before it reached the portion of the process that we designed. This was essential to the design as the massive amounts of carbon dioxide found in the outlet stream significantly affected the flow rates and weight percents of critical items in the outlet streams. In addition to carbon dioxide, it was also assumed that the solid catalyst from the reactor was completely removed by the filtration unit in Yadav's process before the stream reaches our portion of the process such that there are no solids in the streams entering the decanter.

10.1 Separation of Transesterification Reactor Products

The initial portion of the process design focuses on the separation and purification of the streams exiting the transesterification reactor. Although the focus of this design project is to sell the byproducts of the biodiesel production, it is still essential that the biodiesel produced and sold by the design plant we have created follows the industry standards for high-grade biodiesel. Every year the American Society for Testing Materials (ASTM International) releases an updated qualification specification for the sale of biodiesel classified as B100. B100 indicates that the item is sold as 100% biodiesel. At the time of writing, the most current specification for B100 biodiesel is ASTM D6751-18. For our design, the two most important variables to consider were the weight percent of glycerol and methanol in the fatty acid methyl ester mixture. The ASTM distinguishes between two different types of glycerol in their specifications. The first is unreacted glycerol: glycerol still combined with fatty acids in the form of unreacted triglycerides from the transesterification reactor. Since for this design project we were given data assuming a complete reaction during the transesterification process, we are assuming there will be none of this type of glycerin in the product stream. The other type of glycerol specified is free glycerol: reacted glycerol that remains in the stream after the reaction process. The industry standard is less than 0.02% glycerol by weight. The other main critical variable is the amount of methanol in the FAMEs mixture. The ASTM manual states that the amount of methanol in biodiesel cannot exceed 0.2% by weight (ASTM, 2019).

Because of these ASTM requirements, it is essential that the products from the transesterification reactor are separated very well both for the sale of the biodiesel, but also for the sale of glycerin as a byproduct. The first separation process that was chosen was a decanter. The product stream exiting the transesterification reactor is comprised of FAMEs, methanol, and glycerol at 90°C and 50 bar. A decanter was chosen because the exit products of the reactor exist as two immiscible liquid phases because of FAMEs and glycerol limited miscibility with each other. In order to reach as close to the ASTM requirements for B100 biofuel as possible, we chose to run the decanter at 0℃ and 1.379 bar (20 psia). Because glycerol and FAMEs are so similar in boiling point, it is very difficult if not impossible to separate the two items by distillation or a flash vessel, as these processes depend on differences in volatility to create a separation (Science Direct). Therefore, it was essential that as little of the glycerol exiting the reactor as possible ended up in the FAME heavy stream that would eventually become the

product biodiesel. This separation was accomplished by keeping the decanter at a very low temperature and slightly above atmospheric temperature. The resulting FAME stream had only 0.028% glycerol by mass meaning that it was already very close to ASTM requirements.

10.2 Purification of Reactor Products

After their separation into two separate phases, both of the exit streams from the decanter must be purified because of the large amounts of methanol present in both of the streams. The glycerol stream is sent directly to a flash vessel to purify the glycerol in the stream. Because methanol and glycerol have such a large difference in boiling point, it was decided that a separation based on different volatilities would be optimal for their separation. Both a flash vessel and a distillation column were considered for this process. A major consideration for the separation was that glycerol decomposes at 290 °C (Science Direct). Therefore, any separation process must remain well below that temperature. Both a flash vessel and a distillation column were modeled in ASPEN Plus V10 and compared to determine which process was ideal for the separation. A relatively small distillation column with only three trays and running at a reflux ratio of two could separate the glycerol and methanol so well that it would produce a glycerol product stream of 99.99% purity. However, in order for this to occur below the decomposition temperature of glycerol, the column had to be run at a vacuum pressure and therefore would have a larger diameter than a typical distillation column.

The other method considered was a simple flash vessel. The flash, run at 163.8 ℃ and 0.344 bar, was able to selectively separate the glycerol from the methanol while staying below the decomposition temperature. The input specifications for this vessel can be found in the Appendix and the purity of the final glycerol stream as 99.5% by weight. Although lower than the 99.99% purity of the distillation column, most industries consider high-grade glycerol to be any glycerol that is at least 99.5% pure. Therefore, even though it is a lower purity, the glycerol product from the flash vessel can still be sold at the higher market price for clean glycerol (Ahuja, 2018). Also, although the flash vessel must also be run at vacuum pressure, the general costs of a flash vessel, even a vacuum vessel, are still significantly lower than that of a vacuum distillation column. Therefore, it was decided that the flash vessel would be the best choice for the glycerol separation. The resultant streams produce pure product glycerol as well as a methanol stream that will be condensed and recycled to the transesterification reactor.

In addition to the glycerol separation, the FAME stream from the decanter also needs to be purified before the biodiesel can be sold or sent to the Omega-3 separation process. The exit stream of FAME has both glycerol and methanol in it from the reactor. In order to remove the methanol from the stream, it was decided to use a flash vessel. Although a distillation column was also considered, FAMEs, like glycerol, also have a decomposition temperature which was too easily surpassed when designing the distillation column (Science Direct). Instead, a flash vessel was optimized based off of FAME purity requirements to run at 235℃ and 1 bar. It was chosen because this vessel can remove almost all of the methanol in the system as well as continue to reduce the amount of glycerol in the FAME stream. At the conditions of the flash vessel, FAMEs was produced with only 0.024% percent glycerol by mass and 0.25% methanol in the biodiesel stream. Although we were largely able to remove the methanol and glycerol from the FAME product stream their weight fractions in the final product are still very close to the maximum ASTM quality specifications (ASTM, 2019). Because the focus of our project was on isolating the Omega-3s, we did not pursue this area of the project further. However, future research should focus on refining the process suggested here or in finding a different type of separation process that does not depend on volatility to separate the products of the reactor.

Following the separation and purification of the transesterification reactor, four exit streams were produced. The methanol streams from both flash vessels will be condensed and returned to the reactor vessel to be reused in the transesterification process. This process, though simple, is outside the purview of our study. The purified glycerol stream will be collected and sold as a byproduct of the process. The FAMEs are now in a sellable form as biodiesel. Normally in the production of biodiesel, these would be some of the final steps of the plant. However, our focus is on removing the Omega-3 methyl esters from the FAMEs in order to sell them at a higher cost.

10.3 Separation of Omega-3 Methyl Esters from FAME Mixture

Following the purification of the FAMEs produced in the transesterification reactor, the next step in producing higher sale cost byproducts is to separate the methyl ester form of the Omega-3 from the other FAMEs. It is worth noting that algae are incapable of synthesizing fatty acids of a specific length or saturation. This lack of selectivity means that the triglycerides produced can have different fatty acid groups attached to the glycerol group and that there are

many different methyl esters following transesterification. Since this project aims to refine a fraction of these methyl esters selectively, it is important to choose a point to separate the desired Omega-3 methyl esters from other methyl esters. The randomness of the triglycerides coming from the algae prevented this separation from occurring at an earlier step.

The first decision that had to be made for this portion of the plant was how much Omega-3s the plant would produce. Using the *Nanochloropsis salina* strain of algae, the methyl EPA and methyl DHA make up approximately 21% of all of the FAMEs. Our calculations for the first half of the plant found that the plant produces 67,000 kg of FAMEs per hour. If all of the Omega-3s available were removed from the product FAMEs mixture, the amount of Omega-3 produced by this single plant would be more than 50% of the United States market for Omega-3s in 2018. Because of the economic issues that would arise from flooding the market with Omega-3s, it was decided that only a portion of the FAMEs produced at the plant each day would go through the process to separate the Omega-3s. This number was determined by evaluating the projected Omega-3 market in 2024 (Grand View Research, 2014). The plant was then sized such that it could produce up to 30% of the Omega-3 market requirements in that year. This number was found to be 1375 kg/hr of EPA and DHA in their carboxylic acid form. The amount of FAMEs required to produce the goal amount of EPA and DHA per hour was determined using 1375 kg/hr of EPA and DHA as the target goal. It was found that 7625 kg/hr of FAMEs was required to be separated in order to reach the goal production of Omega-3s. Therefore, following the purification of the FAME stream, a splitter was added into the process to divert a small percentage of the product FAMEs to the Omega-3 separation process. The remaining FAMEs not diverted to the Omega-3 process will be sent directly to storing and shipping and be sold as biodiesel.

Choosing a separation process to separate Omega-3 methyl esters from others was nontrivial due to the similar chemical properties that these compounds have. Initial ideas of using a separation process based on boiling points, i.e., distillation or flash, were quickly discarded due to how high the boiling points were for the methyl esters found in the literature. The concern stems from the likelihood that the compounds would thermally degrade before vaporizing, and from how similar the boiling points were between the compounds. Crystallization was also considered since then and has been performed (Chen, 2001), but the sub-zero melting points of these compounds were an immediate concern due to refrigeration costs. The lack of literature

regarding how these molecules crystallize and the necessity of using additives such as urea quickly translated to worries that pursuing this route would create an inseparable slurry (Pando, 2018). Since these two methods were unviable for this design, a search for a different and novel separation technique capable of performing the desired separation was necessary.

After an extensive amount of research into the topic, we returned to the most commonly used method to separate FAMEs: chromatography. Chromatography had several issues for us mainly that it was not a continuous process because of the necessary elution step, and it is generally run for very small amounts of liquid. Since our plant planned to process almost 8000 kg of FAMEs per hour, an actual chromatography column was not feasible. However, a common focus of FAME chromatography is using ionic liquids to complex with more highly unsaturated methyl esters (Cheong et al. 2011; Dolowy and Alina, 2015). Through even more research, a handful of papers were found on utilizing the same type of complexation in liquid-liquid extraction for larger scale separations (Li et al. 2009; Xing et al., 2014). The lower energy requirements and the very high selectivities motivated the use of a liquid-liquid extraction to separate the heavier unsaturated methyl esters. The LLE uses the same basic principles as the chromatography column but uses absorption instead of adsorption for the separation process.

One advantage we had was that the most unsaturated fatty acids that *N. salina* was likely to produce were the desired Omega-3 fatty acids. The remaining fatty acids can vary in length and have the same number of carbons as the Omega-3 fatty acids but were unlikely to have as many double bonds. For this process, the FAMEs stream will be run in a countercurrent column against a solution of silver nitrate in methanol. Silver Nitrate is used for the process because research has shown that the free silver ions in the solution complex with pi bonds (Teramoto, 1994). Pi bonds are the bonds formed in double or triple bonds in a chemical compound. Not only does the silver only complex to double bonds, but it has been shown that it selectively binds to the compounds with the most pi bonds first. This selectivity means that the silver nitrate will only bond with FAMEs that are unsaturated and selectively bonds to the most unsaturated first. Because the methyl EPA and DHA have five and six double bonds respectively, while the other unsaturated FAMEs have at most three, the silver ions from the silver nitrate will very selectively complex with only the methyl EPA and methyl DHA.

A lot of more recent research has focused on specifically Ionic Liquids for this process (Li, 2016). These are specifically formulated, highly expensive solutions that do work very well

for this process. However, after reviewing the literature, we found that the slightly higher purity and selectivity available from the ionic liquids did not compare to its significantly higher cost, especially because it had been shown that the LLE would also work just using silver nitrate.

Although the silver nitrate can simply be dissolved in water and will still complex well with the methyl Omega-3s, research has shown that the partition coefficient of the LLE increases by a factor of 1000 when 100% methanol is used instead of either pure water or a mixture of water and methanol (Teramoto et al., 1994). Using methanol therefore significantly reduces the amount of solvent required for the LLE process, and also reduces the residence time required in the columns. The first of the two columns will be a countercurrent column that will flow FAMEs against the silver nitrate methanol solution. Luckily, no organic solvent is required for the FAME mixture. Although lab-scale experiments frequently dissolve FAMEs in hexane before experiments, several papers have tested separations using FAMEs without a solvent with much success (Li et al., 2009; Teramoto et al., 1994). Therefore, in order to reduce costs, using no solvent allows this process to run without an additional separation unit as well as the overhead cost of purchasing the hexane solvent for the FAMEs. The LLE column was designed so that the liquids in the column would have a residence time of at least 25 minutes as this was found to be the optimal amount of time for mixing in order for the maximum amount of Omega-3s to move into the Silver solution (Li et al., 2009).

Because the free silver ions from the first LLE complex to the methyl EPA and DHA, the mixture must be run through an additional liquid-liquid extraction instead of simply being separated based on volatility or differences in other types of properties. Similar to the elution process in chromatography columns, the silver nitrate methanol solution now containing the methyl EPA and DHA will enter a second countercurrent column that will be run against a stripping agent: 1-hexene. Both 1-hexene and diethyl ether are excellent stripping agents for complexed silver methyl EPA and DHA (Xing, 2014). However, because this plant is at an industrial scale, safety must be our first consideration. Diethyl ether, although an excellent stripping agent, is quite unsafe as its highly volatile and can even be used as a fire starter or accelerant. Therefore, it was decided that 1-hexene would be used as the stripping solvent in the second LLE. The column was designed with a residence time of 10 minutes based on extraction research (Li et al., 2009) and uses enough 1- hexene to ensure that there is more than enough 1-hexene for all of the Methyl EPA and DHA to move into the 1- hexene phase. Most research

found that the exit stream of the LLE would have at maximum 50% methyl EPA DHA and 50% 1-hexene by weight. Therefore, the LLE was designed with enough 1-hexene such that if 100% of the FAMEs moved from the silver nitrate methanol solution to the hexene phase, the methyl EPA and methyl DHA would make up only 45% by mass of the final exit stream.

The final step of the separation of the methyl Omega-3s from the FAMEs stream is to separate the methyl EPA and methyl DHA from the organic stripping solvent 1-hexene. This is a relatively easy process because the difference in boiling point between 1-hexene and the long chain species is over 300 °C (Science Direct). Therefore, it was decided that a flash vessel was more than capable of separating the 1- hexene from the methyl esters. In order to reduce the 1-hexene in the methyl ester stream to below 1%, the flash vessel was optimized to run at a temperature of 107℃ and a pressure of 0.133 bar. Although this is once again a vacuum vessel, the low pressure was essential to keeping the separation temperature below the decomposition temperature of the methyl EPA and DHA and to not lose significant amounts of the methyl Omega-3s in the hexene stream off the top of the vessel. The 1-hexene will be condensed and then recycled to the second of the two liquid-liquid extractions.

10.4 Hydrolysis of FAMEs to Free Fatty Acids

Raw Omega-3 material is sold in a carboxylic acid, or free fatty acid form. Since the product emerging from the liquid-liquid extractions described previously are still methyl esters, the remainder of the design needs to hydrolyze these compounds to acids. While the literature for methyl ester hydrolysis is scarce, the hydrolysis of triglycerides and other esters is better studied, and extrapolations can be made from those reactions. In general, this hydrolysis can be acid-catalyzed or base-catalyzed (Ma, 1999). However, the acid-catalyzed route generally requires longer reaction times and additional catalysts to obtain the yields that the base-catalyzed route does (Jiménez et al., 2010). Thus, base-catalyzed hydrolysis based on the work performed by Kandula on ethyl ester hydrolysis was selected for this process (Kandula, 2018).

Initial research about Omega-3 fatty acids revealed that these compounds are prone to oxidation. As a result, all vessels planned in this step are expected to maintain an inert atmosphere and will necessitate purchasing nitrogen gas as a capital cost to do so. Additionally, the equipment in this portion of the process will be made of 304-stainless steel unless mentioned

otherwise. This choice of material is due to the corrosive conditions being applied, stemming from the use of strong acids and bases to perform the desired chemistry (Jacobsen et al., 2013).

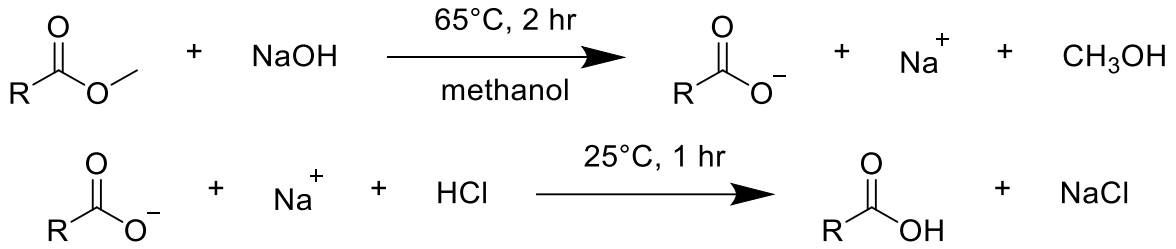


Figure 10.1 Reaction of FAME to FFA. A methyl ester attached to a fatty acid (R) group is converted to a fatty acid carboxylate through the addition of NaOH. The carboxylate is converted to the fatty acid with the addition of HCl.

The base-catalyzed reaction first requires reacting the FAMEs with a base to form the fatty acid carboxylate and methanol. The carboxylate will later react with an acid to form the desired carboxylic acid and an aqueous salt based on the acid and base used. These steps are summarized in Figure 10.1. Kandula's hydrolysis of an ethyl ester used sodium hydroxide (NaOH) as the base and hydrochloric acid (HCl) as the acid (Kandula, 2018), and formed sodium chloride (NaCl) as the salt. Potassium hydroxide (KOH) was another candidate for the base upon recommendation from both consultants and the literature (Salimon et al., 2011). Potassium chloride (KCl), or the muriate of potash, is a known fertilizer and could potentially be sold to recoup some of the costs of building this plant ("Potassium Chloride"). These potential cost savings were not thoroughly explored in this proposal since the KCl produced in this process would have been in aqueous solution and require desalination to be sold as fertilizer. Investigating the costs associated with designing a desalination plant revealed that this would not have been simple nor inexpensive (Mishra, 2018). Additionally, the cost of KOH is $200/metric-ton more than NaOH. Therefore, this design did not select using KOH as the base.

Design of the reactor to perform the first base-addition step was initially based on Kandula's hydrolysis (Kandula, 2018). This step involves adding NaOH, frequently purchased in aqueous solution, to a low-density organic immiscible with water. Methanol is added and serves as a solvent miscible with FAMEs and the aqueous phase to promote the reaction. At this point, work by Salimon, Kywe, and Berchmans was consulted to determine the amounts of solvent and NaOH needed as a direct scaling up of Kandula's work would have required a large amount of solvent and the design of oversized reactors. Work done on the hydrolysis of *Jatropha curcas* oil led to the selection of adding 6 molar equivalents of methanol per mole of FAME and the addition of 1.2 molar equivalents of NaOH per mole of FAME to promote the base-reaction

equilibrium towards forming a stoichiometric amount of carboxylate (Salimon et al., 2011; Kywe & Mya, 2009; Berchmans & Shizuko, 2008). Salimon and Kywe also concluded that this reaction had the best hydrolysis yields when operating for 2 hours at 65°C and atmospheric pressure, and these conditions were applied for designing the two stirred tank reactors in series that would be used to carry out this chemistry. The design of two tanks in series, each with a residence time of 1 hour, was intended to maximize the likelihood that materials would stay within this step for the desired residence time of 2 hours.

The FAME stream coming from the previous section, aqueous NaOH, and methanol were all added to the first reactor. Since the FAMEs coming from the flash are coming at high temperatures, heat needs to be removed from these reactors over time. Fortunately, the surface area of each reactor is large enough to purchase water jackets which allow for heat exchange with cooling water. NaOH can be purchased as a 50 wt% solution in water, and this process will dilute it with extra process water in a separate storage tank before addition to the reactor. Using NaOH lowers the temperature of the contents in the reactors and ensures that all the reactor contents stay liquid and do not vaporize.

Following the formation of the carboxylate, the stream exiting the second base-reaction stirred tank reactor enters a distillation tower. The distillation aims to reduce the volume of material entering the acid-reaction step to follow and to recover a large amount of methanol. This methanol can then be recycled back as a solvent for the base-reactors. While a flash vessel could be used instead of a distillation tower, there were two factors to consider. The first factor is stoichiometric: there is expected to be more methanol leaving the base-reactors than entering due to the reaction to form the carboxylate. Therefore, there would either need to be the choice of higher volumes entering the acid reactor, or a need to flash more methanol that could be used as a solvent. The second factor is that the triglyceride transesterification reactor in the Yadav process consumes methanol, and excess methanol being separated by distillation could be used to help offset the methanol requirements of this reactor. This step requires a high purity of methanol, and distillation can reduce the concentration of water in the distillate methanol stream sufficiently for the Yadav step. Thus, a distillation tower was chosen to separate methanol which could be recycled to previous steps and to reduce the volume of the stream that needs further processing to form the Omega-3 product.

As an aside, it is noted that the methanol distillate exits at a high temperature. After splitting off the excess distillate that can be sent to the transesterification reactor, the methanol to be recycled back to the base-reaction reactors is still at a high temperature. Immediately sending it at this high temperature would significantly increase the heat removal demands of the base-reaction reactors and a more complex shell-and-tube heat exchanger would need to be built. Instead of building a heat exchanger for the base-reaction reactors, it is simpler to remove heat from the methanol distillate before it enters the reactor. One advantage is that it is conceptually more straightforward: rather than cycling an arbitrary amount of the contents from the base-reaction reactors through a heat exchanger, the flow rate of methanol that needs to be cooled can be calculated by Aspen. Another advantage is the material of the heat exchanger: a strong base like NaOH could corrode the heat exchanger and require stainless steel as the tube material, while there is no fear of this corrosion with methanol with cheaper carbon steel for the tubes. Modeling this recycle in Aspen was not perfect since the software needed to start with a flow of methanol. Thus, the Aspen flowsheet had a separate methanol inlet stream to the NaOH-reactor and had this recycle stream modeled as an outlet to leave the system. The simulation was run once to obtain the composition of the recycle stream. The results of this first iteration were the values used for the inlet methanol stream. As a result, the stream results to be presented in Section 12.4 will be imperfect but will give a close idea of the expected compositions.

The bottoms of the distillation tower are sent to an acidification step, where the carboxylates can react with hydrochloric acid (HCl) to form the desired Omega-3 fatty acid in a carboxylic acid form and water. Additionally, the sodium cations and chloride anions in this vessel can form NaCl, but these ions are likely to be solvated in water. Both Kandula and Salimon claimed to add enough HCl to attain a pH of 1. Extrapolation from this data led to the selection of a residence time of 1 hour and reaction conditions of room temperature and atmospheric pressure. Additionally, 1.3 molar equivalents of HCl were added per mole of fatty acid carboxylate. This was chosen based on the stoichiometric amounts of carboxylate, and hydroxide ions present coming from the distillation in order to promote equilibrium towards forming the desired fatty acids. Additional process water is also added to the reactors. In this case, the main concern is keeping all the NaCl solubilized in the liquid phase and preventing the accumulation of solids in the reactor. As in the base-reaction step, the equipment for this acid-

reaction step will use two stirred tanks in series to promote the amount of material that stays in this step long enough to reach the desired residence time.

The stream exiting the acid step is expected to exist in two phases: a light-oily liquid phase consisting of the Omega-3s and a heavy-aqueous phase consisting of water, excess acid, and NaCl salts. An assumption was made at this step that the two phases would be completely immiscible, and this seems reasonable since the Omega-3s are very long linear hydrocarbons. Thus, a decanter is expected to be capable of separating the two phases. Unfortunately, modeling this process in Aspen with a Decanter block was unsuccessful due to the lack of partition coefficient data, either in the literature or from using Aspen to calculate a value using UNIFAC. One reason for this failure may be due to the small difference in density between the two phases, which is approximately 0.05 kg/L. From a design perspective, a workaround for a poor density difference would be to model the decanter with a minimum residence time of 30 minutes and with a length-to-diameter ratio of least 3. The second reason for this failure could be the minute amounts of methanol and hexene which remain in the stream. It is possible that these organic solvents may prevent the Omega-3s from emerging from the decanter as pure as this design may require. Additionally, the small presence of methanol, which is expected to be miscible with the FAMEs as well as water, may be enough to prevent two phases from forming. While more research and experiments would be required to confirm if these concerns are warranted, an alternative separation process would be required if the assumption of having two separable liquid phases at this step does not hold.

Some research into alternative processes led us to consider a liquid-liquid extraction because of the potential issues with the decanter. Research has been performed, primarily with octanol and heavy organic solvents, on how carboxylic acids can be extracted and subsequently separated from the extractant solvent by using a flash vessel (Sangster, 1989). The results of these studies cannot be applied directly to this process because the carboxylic acids studied are more volatile than the extractants. However, there is also literature on how heptane can be used as an extracting solvent, and separation of heptane and the Omega-3s by vacuum distillation is theoretically possible (Goodman, 1958; Simpson, 1974). The hesitation in approaching this step, however, is the obvious increase in capital cost that would result from designing the equipment and the lack of available literature to inform how this liquid-liquid extraction would perform on an industrial scale. Therefore, a decanter is what this process will use to separate the Omega-3

fatty acids from the other components and the separation will be modeled in Aspen using a Sep block. The two streams exiting the decanter can then be sent to a storage tank where they can be held until they are sold or sent away.

One final detail to take care of is the treatment of the aqueous phase exiting the decanter. This stream will still be acidic due to the small excess of HCl added. Additionally, there will be small amounts of organic compounds, i.e., methanol and 1-hexene, and a high concentration of salts. Sending this water back to a treatment plant or the algal raceways were both considered. In either case, however, it is common practice to first neutralize the acidity of the wastewater stream before further waste treatment handling (Seider et al., 2017). This neutralization can be accomplished by adding a stoichiometric amount of NaOH relative to the amount of HCl present in the stream. After neutralizing the water, each of the two proposed ideas of how to dispose of this waste stream can be considered.

The presence of organic compounds in the waste stream may require further water treatment before being released to an open body of water. Thus, one way to address this waste is to have it stored in a storage tank until it can be sent to a treatment facility which specializes in wastewater treatment (Clean Harbors). The main cost associated with this would be the cost of treating the organic compounds. If this water were to be sent back to the algal raceways, the salinity of the water would need to decrease. *N. salina* is a species of algae which grows in salt water, which has a salinity of 3.5 g salt/L (USGS). This amount is much lower than the concentration of salt that Aspen predicts to be present in the waste stream. Thus, the waste stream either needs to be desalinated or diluted. Since desalination was already a cost concern earlier, this option was not pursued. Diluting the stream would require large amounts of water, but the literature suggests that supplying algae with certain amounts of organic material can promote algal growth (Miazek et al., 2017). Thus, there would not need to be any treatment of organic material if the water could be sent to the algal raceways. Unfortunately, part of the processing of algae that is out of scope for this project already accounts for supplying the algal raceways with enough water. Additionally, some calculations done showed that it would be cheaper to have the water treated rather than return it to the raceways (Appendix). As a result, this design process will assume that the wastewater will be sent to a treatment plant and that the main cost will be the cost of treatment of organic material, which will be assumed to be $0.15/lb organic (Seider et al., 2017, p. 500).

11. Assembly of Database

11.1 Aspen Plus Modeling

A large portion of this process was modeled using the Aspen Plus software. However, Aspen's database did not have all the property values required to model the entirety of the process. In many cases, Aspen estimated variables that were not known in the chemical database and these estimations were sufficient to obtain results. The processes designed in Section 10.1 (Separation of Transesterification Reactor Products) and Section 10.2 (Purification of Reactor Products) used the RK-SOAVE method to calculate molecular properties because the non-FAME materials were known compounds (e.g., glycerol). Meanwhile, the process designed in Section 10.4 (Hydrolysis of FAMEs to Free Fatty Acids) used the ELECNRTL due to the ionic species that were present as a result of the acid-base chemistry that was required. FLASH2 blocks were used to model flash distillation vessels. RADFRAC blocks were used to model distillation towers. HEATX blocks were used to model the cooling or heating of streams, which had not already been performed within a RADFRAC block. RSTOIC blocks were used to model the chemical reactions using the FAMEs as a limiting reagent since the stoichiometry of reactions was known.

The only processes not at least partially modeled in Aspen were the two liquid-liquid extraction columns. Aspen had very limited solubility data for methyl EPA, the methyl DHA, and the extractant silver nitrate mixture. The calculations for these LLEs were performed in Excel, and these calculations can be found in the appendix in Section 25.2.3 The Aspen reports are also available and can be found in Section 25.4.

11.2 Feed Stream Composition

The work performed by Yadav modeled all inlet FAMEs as methyl oleate, a C18:1 FAME (Yadav et al., 2019). While that may have been satisfactory for the work the group did on biodiesel production, it is insufficient for this process which cannot assume that there is a uniform FAME stream. The work of Ma and Marudhupanti were reviewed to establish the composition of the product stream from Yadav's transesterification reactor (Ma et al., 2014; Marudhupanti et al., 2016). Both had studied the fatty acid composition of *N. salina* after hydrolyzing the triglycerides that were produced and determined a certain average composition

of fatty acids present for a total of four strains of *N. salina*. Ma's work utilized two different strains of *N. salina* grown under similar conditions while Marudhupanti's work cultivated *N. salina* under different growing conditions. There were three classifications of FAMEs that could be made across their work: saturated fatty acids (no double bonds), monounsaturated fatty acids (one double bond), and polyunsaturated fatty acids (more than one double bond). The FAME inlet composition for this process was composed by averaging the compositions observed by Ma and Marudhupanti and identifying the most populous species (i.e., species whose presence was greater than 10 mol%). An exception was made for DHA because it is an Omega-3 acid and stearic acid (C18:0) to contribute to the diversity of saturated fatty acids and the presence of 18-carbon FAMEs present in the stream. The mass contributions of less populous species were captured by selecting representative molecules from each category (i.e., C14:0, C18:1, C18:2). These were selected because they were the most populous species remaining in each of these categories. The results are summarized in Table 11.1.

Table 11.1 Composition of Inlet FAME

Species	Mol%
C14:0	7.28
C16:0	31.95
C16:1	17.17
C18:0	2.10
C18:1	14.67
C18:2	7.80
C20:5 (EPA)	17.90
C22:6 (DHA)	1.13

11.3 FAME Properties

Table 11.2 compiles information listed in SciFinder that was experimentally collected about the fatty acid methyl esters in this process. The main conclusions that could be drawn about these compounds are that the boiling points of FAMEs are very high, the melting points of FAMEs are low, and that these are oily compounds with a lower density than water.

Table 11.2 Properties of FAMEs at 1 Atmosphere

Compound	Equivalent Lipid No.	Molecular weight (g/mol)	Boiling point	Melting point	Specific gravity (20°C)
Palmitic acid methyl ester	C16:0	270.45	319 - 321 °C	32 - 35 °C	0.865±0.06 (predicted)
Palmitoleic acid methyl ester	C16:1	268.43	394.2±0.0 °C (predicted)	-0.5 - 0.5 °C	0.876±0.06 (predicted)
Stearic acid methyl ester	C18:0	298.50	370 °C	37 - 41 °C	0.8643
Oleic acid methyl ester	C18:1	296.49	351.4±0.0 °C (predicted)	-19.9 °C	0.8739
Eicosapentaenoic acid methyl ester (EPA)	C20:5	316.48	402.8±34.0 °C (predicted)	N/A	0.912±0.06 (predicted)
Docosahexaenoic acid methyl ester (DHA)	C22:6	342.51	429.9±24.0 °C (predicted)	N/A	0.917±0.06 (predicted)

11.4 Raw Material Costs

The cost of each raw material was determined using several different databases. The methanol price was determined using the website Methanex which delivers updated prices for methanol in varying markets. The price used was for the United States market in 2019. The other values were estimated by viewing ranges of bulk prices on Alibaba to determine the average price for our product. The costs used for all of the raw materials in the process are listed below in Table 11.3.

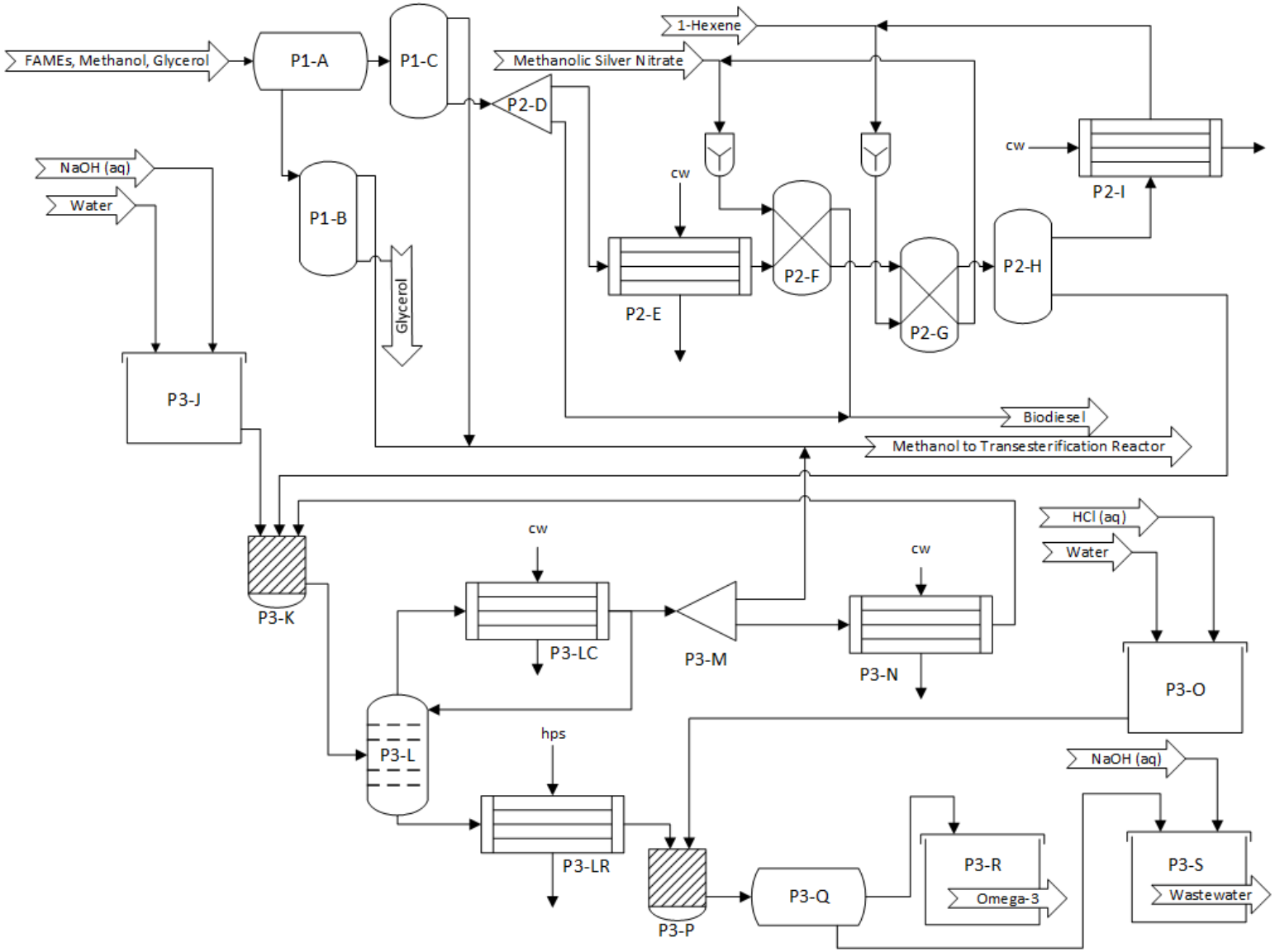
Table 11.3 Raw Material Costs for Process

Material	**Cost**	**Units**
1- Hexene	$1.45	per kg
NaOH	$0.30	per kg
HCL	$0.10	per kg
Silver Nitrate	$400.00	per kg
Methanol	$432.00	per metric ton
Nitrogen	$65.00	per l at 200 bar

12. Process Flow Diagram and Material Balances

The process flow diagrams presented in the figures below illustrate the proposed process for the separation of the methyl Omega-3s and their conversion to the carboxylic acid form. Figure 12.1 is an overview of the process that shows the main blocks and streams in the plant. Figure 12.2 and Table 12.1 illustrate part 1 of the process. This part includes the separation of the products from the transesterification reactor and their purification using flash vessels. Figure 12.3 and Table 12.2 illustrate part 2 of the process. These figures show the separation of the methyl Omega-3s from the other FAMEs using LLE and their purification. Figure 12.4 and Table 12.3 are part 3 of the process and illustrate the process of converting the methyl Omega-3s from their methyl ester form to their carboxylic acid form. Associated tables outlining the streams and their compositions are also included.

12.1 Overall Process Diagram



P1-A	FAME-Glycerol-Methanol Decanter
P1-B	Glycerol-Methanol Flash Vessel
P1-C	FAME-Methanol Flash Vessel
P2-D	FAME Splitter
P2-E	FAME Cooler
P2-F	FAME-Silver LLE
P2-G	FAME-Hexene LLE
P2-H	FAME-Hexene Flash Vessel
P2-I	Hexene Condenser
P3-J	NaOH Tank
P3-K	NaOH Reactor
P3-L	Omega-3-Methanol Distillation
P3-M	Methanol Splitter
P3-N	Methanol Cooler
P3-O	HCl Tank
P3-P	HCl Reactor
P3-Q	Omega-3-Water Decanter
P3-R	Omega-3 Storage
P3-S	Water Neutralization/ Storage

Figure 12.1. Overall Process Diagram This flowsheet demonstrates the main streams and blocks in the process of purifying the transesterification reactor products into biodiesel, 99.5% purity glycerol and Omega-3 carboxylic acids. The blocks are labeled by their part of the process. The definition of each block can be found to the right of the diagram, and the details are in Section 15.

12.2 Separation of Transesterification Reactor Products Process Diagram

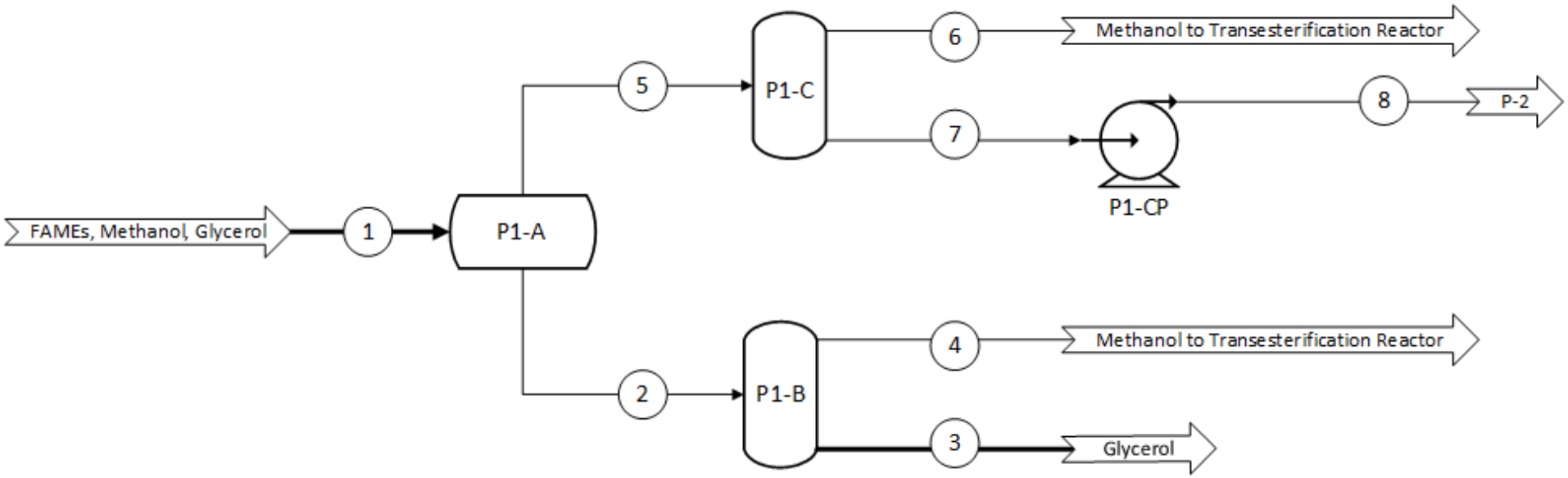


Figure 12.2 Process flow diagram of part 1 of the system. This includes the separation of transesterification reactor products using a decanter, and the purification of both glycerol (P1-B), and FAMEs (P1-C) streams. Banner arrows indicate streams entering or exiting the diagram. Thick, bolded lines indicate a flow stream in or out of the entire process.

Table 12.1 Part 1-Separation of Transesterification Reactor Products Stream Report

Stream ID	1	2	3	4	5	6	7	8
Temperature (°C)	90	0	163.8	163.8	0	235.4	235.4	235.4
Pressure (Bar)	50	1.3790	0.3447	0.3447	1.3790	1	1	1.2
Vapor Fraction	0	0	0	1	0	1	0	0
Total Flow (kg/hr)	77858.3	9562.4	4546.4	5016.0	68295.9	1745.6	66550.4	66550.4
Component Flow (kg/hr)								
C14:0-ME	4178.3	0	0	0	4178.3	128.9	4049.4	4049.4
C16:0-ME	20461.3	0	0	0	20461.3	305.4	20155.9	20155.9
C16:1-ME	10909.9	0	0	0	10909.9	153.5	10756.5	10756.5
C18:0-ME	1493.1	0	0	0	1493.1	10.7	1482.4	1482.4
C18:1-ME	10295.1	0	0	0	10295.1	71.7	10223.3	10223.3
C18:2-ME	5436.8	0	0	0	5436.8	38.1	5398.7	5398.7
EPA-ME	13415.2	0	0	0	13415.2	27.5	13387.7	13387.7
DHA-ME	912.4	0	0	0	912.4	0.8	911.6	911.6
Methanol	5493.3	4319.2	20.3	4298.9	1174.1	1005.1	169.0	169.0
Glycerol	5263.0	5243.2	4526.2	717.0	19.8	3.8	16.0	16.0

12.3 Separation of Omega-3 Methyl Esters from FAME Mixture Process Diagram

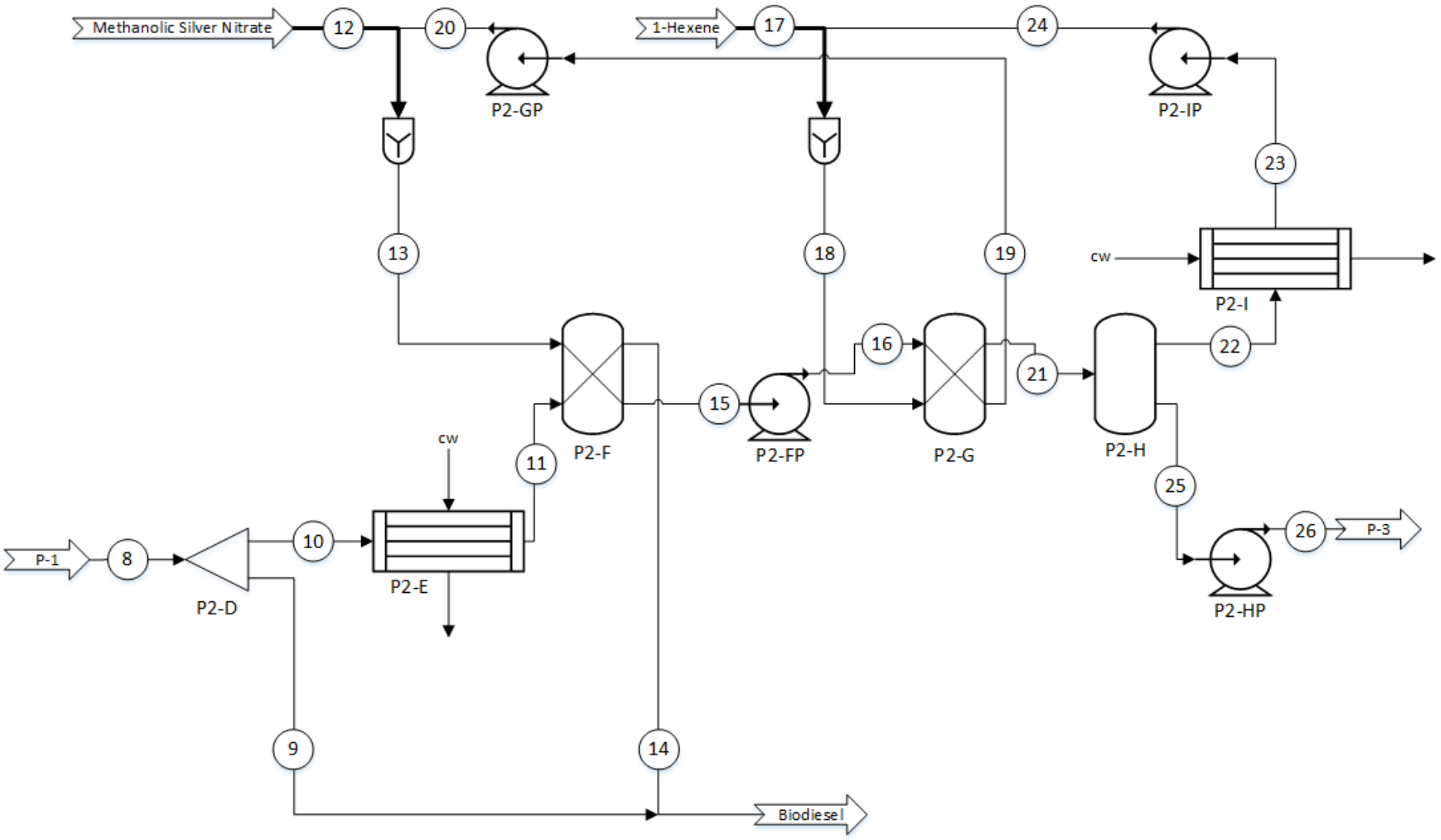


Figure 12.3. Process flow diagram of part 2 of the system. This includes splitting the FAMEs into products and a stream to send to the Omega-3 process. It also includes the separation of the methyl Omega-3s from the FAMEs by two LLE processes (P2-F, and P20-G), and the methyl Omega-3s removal from 1-hexene using a flash vessel. Banner arrows indicate streams entering or exiting the diagram. Thick, bolded lines indicate a flow stream in or out of the entire process.

Table 12.2 Part Two-Separation of Omega-3 Methyl Esters from FAME Mixture Stream Report

Stream ID	8	9	10	11	12	13	14	15	16	17
Temperature (°C)	235.4	235.4	235.4	35	35	35	35	35	35	35
Pressure (Bar)	1.2	1.2	1.2	1.1	1	1.1	1	1	1.1	1
Vapor Fraction	0	0	0	0	0	0	0	0	0	0
Total Flow (kg/hr)	66550.4	58923.7	7626.7	7626.7	0	9204.8	6185.0	10644.8	10644.8	16.5
Component Flow (kg/hr)										
C14:0-ME	4049.4	3585.4	464.1	464.1	0	0	464.1	0	0	0
C16:0-ME	20155.9	17846.0	2309.9	2309.9	0	0	2310	0	0	0
C16:1-ME	10756.5	9523.8	1232.7	1232.7	0	0	1233	0	0	0
C18:0-ME	1482.4	1312.5	169.9	169.9	0	0	169.9	0	0	0
C18:1-ME	10223.3	9051.7	1171.6	1171.6	0	0	1172	0	0	0
C18:2-ME	5398.7	4780.0	618.7	618.7	0	0	618.7	0	0	0
EPA-ME	13387.7	11853.4	1534.2	1534.2	0	0	1534	1518.6	1518.6	0
DHA-ME	911.6	807.1	104.5	104.5	0	0	104.5	103.4	103.4	0
Methanol	169.0	149.6	19.4	19.4	0.13	4954.3	19.36	4954.3	4954.3	0
Glycerol	16.0	14.2	1.8	1.8	0	0	1.84	0	0	0
Water	0	0	0	0	0	0	0	0	0	0
Silver Nitrate	0	0	0	0	0.15	4250.5	0	4250.5	4250.5	0
1- Hexene	0	0	0	0	0	0	0	0	0	16.5

Stream ID	18	19	20	21	22	23	24	25	26
Temperature (°C)	35	35	35	35	106.9	35	35	106.9	106.9
Pressure (Bar)	1.1	1	1.1	1	0.1333	1	1.1	0.1333	0.1333
Vapor Fraction	0	0	0	0	1	0	0	1	1.2
Total Flow (kg/hr)	3200.6	9204.5	9204.5	4640.9	3184.1	3184.1	3184.1	1456.8	1456.8
Component Flow (kg/hr)									
C14:0-ME	0	0	0	0	0	0	0	0	0
C16:0-ME	0	0	0	0	0	0	0	0	0
C16:1-ME	0	0	0	0	0	0	0	0	0
C18:0-ME	0	0	0	0	0	0	0	0	0
C18:1-ME	0	0	0	0	0	0	0	0	0
C18:2-ME	0	0	0	0	0	0	0	0	0
EPA-ME	0	170.1	170.1	1349	0.379	0.3791	0.3791	1348.1	1348.1
DHA-ME	0	11.6	11.6	91.82	0.0058	0.0058	0.0058	91.8	91.8
Methanol	0	4954.3	4954	0	0	0	0	0	0
Glycerol	0	0	0	0	0	0	0	0	0
Water	0	0	0	0	0	0	0	0	0
Silver Nitrate	0	4250.5	4251	0	0	0	0	0	0
1- Hexene	3200.6	0	0	3201	3183.722	3183.7	3183.7	16.9	16.9

12.4 Hydrolysis of FAMEs to Free Fatty Acids Process Diagram

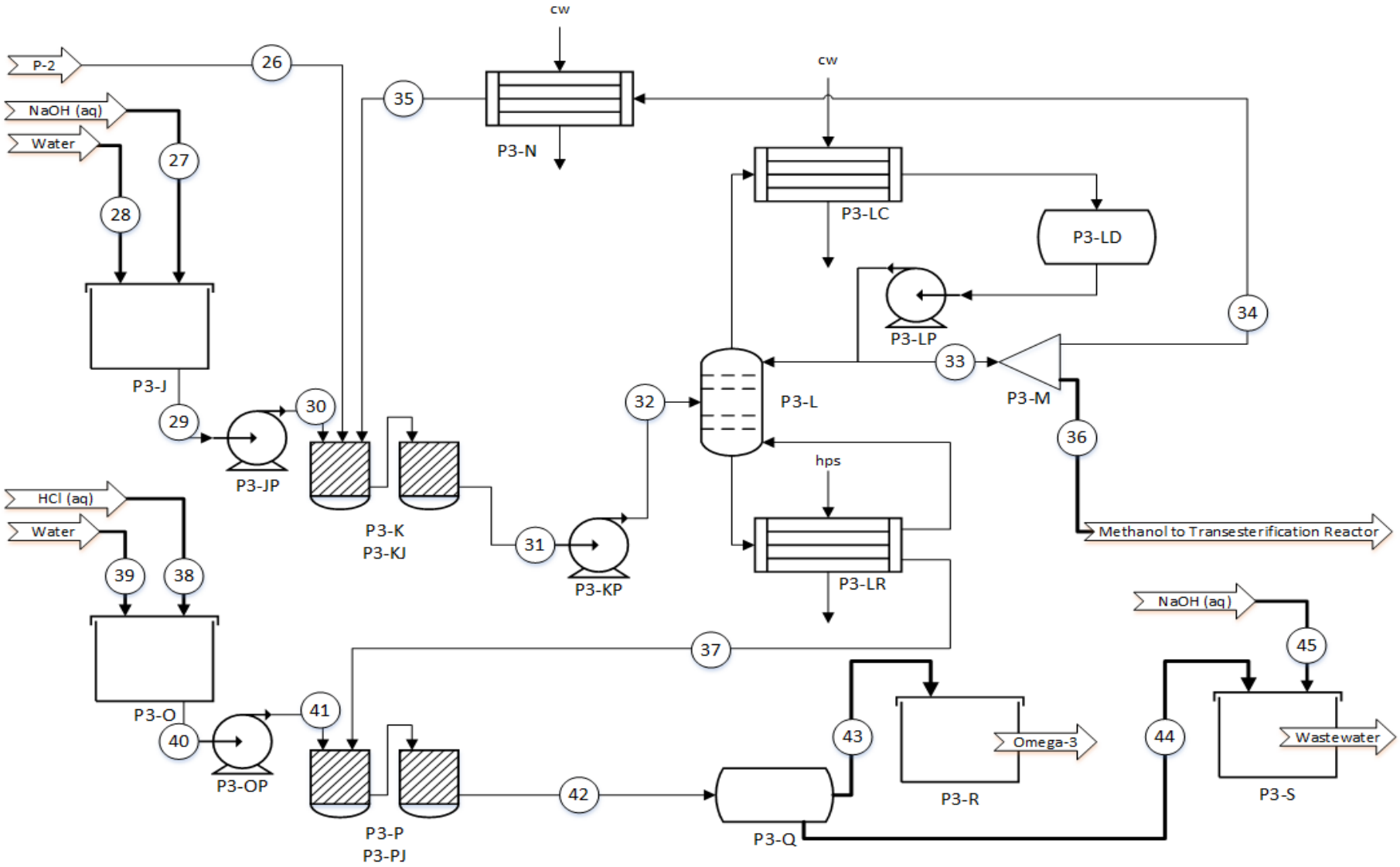


Figure 12.4. Process flow diagram of part 3 of the system. This includes the formation of fatty acid carboxylate using sodium hydroxide in stirred tanks, recycle of methanol by distillation, formation of desired fatty acid using hydrochloric acid, and the separation of two liquid phases using a decanter. Banner arrows indicate streams entering or exiting the diagram. Thick, bolded lines indicate a flow stream in or out of the entire process.

Table 12.4 Part Three-Hydrolysis of FAMEs to Free Fatty Acids Stream Report

Stream ID	26	27	28	29	30	31	32	33	34	35
Temperature (°C)	107.0	25.0	25.0	54.5	54.5	65.0	65.1	74.9	74.9	35.0
Pressure (Bar)	1.20	1.01	1.01	1.01	1.21	1.01	1.80	1.50	1.50	1.50
Vapor Fraction	0	0	0	0	0	0	0	0	0	0
Total Flow (kg/hr)	1439.41	434.05	595.11	1029.16	1029.16	3341.50	3341.50	1014.47	873.91	873.91
Component Flow (kg/hr)										
EPA-ME	1346.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DHA-ME	91.57	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na-EPA Carboxylate	0.00	0.00	0.00	0.00	0.00	1380.25	1380.25	0.00	0.00	0.00
Na-DHA Carboxylate	0.00	0.00	0.00	0.00	0.00	93.70	93.70	0.00	0.00	0.00
EPA	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DHA	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water	0.00	217.02	595.11	812.14	812.14	814.59	814.59	2.85	2.46	2.46
Methanol	0.00	0.00	0.00	0.00	0.00	1014.18	1014.18	1009.11	869.29	869.29
1-Hexene	1.43	0.00	0.00	0.00	0.00	2.61	2.61	2.51	2.16	2.16
NaOH	0.00	217.02	0.00	217.02	217.02	36.17	36.17	0.00	0.00	0.00
HCl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NaCl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Stream ID	36	37	38	39	40	41	42	43	44	45
Temperature (°C)	74.9	127.5	25.0	25.0	36.8	36.9	25.0	25.0	25.0	25.0
Pressure (Bar)	1.50	1.71	1.01	1.01	1.01	1.60	1.20	1.20	1.20	1.01
Vapor Fraction	0	0	0	0	0	0	0	0	0	0
Total Flow (kg/hr)	140.55	2327.03	714.09	157.95	872.04	872.04	3199.08	1374.55	1824.52	35.97
Component Flow (kg/hr)										
EPA-ME	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DHA-ME	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na-EPA Carboxylate	0.00	1380.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na-DHA Carboxylate	0.00	93.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EPA	0.00	0.00	0.00	0.00	0.00	0.00	1286.73	1286.73	0.00	0.00
DHA	0.00	0.00	0.00	0.00	0.00	0.00	87.82	87.82	0.00	0.00
Water	0.40	811.74	499.86	157.95	657.81	657.81	1485.85	0.00	1485.85	17.98
Methanol	139.81	5.07	0.00	0.00	0.00	0.00	5.07	0.00	5.07	0.00
1-Hexene	0.35	0.11	0.00	0.00	0.00	0.00	0.11	0.00	0.11	0.00
NaOH	0.00	36.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	17.98
HCl	0.00	0.00	214.23	0.00	214.23	214.23	16.39	0.00	16.39	0.00
NaCl	0.00	0.00	0.00	0.00	0.00	0.00	317.11	0.00	317.11	0.00

13. Process Descriptions

The process begins with the stream (labeled as stream 1 in Figure 12.2) comprised of FAMEs, methanol, and glycerol from the transesterification reactor. Several assumptions were made about the products of the transesterification reactor. Before our process, it is assumed that all of the catalyst used in the reactor has already been removed from the stream. Since it is a solid catalyst it will be filtered out. However, this process is outside of the bounds of our project. Also, it is assumed that all of the carbon dioxide from the oil separation and the reactor has already been vented off in the system such that there is no carbon dioxide gas present or any carbon dioxide dissolved into the liquid stream exiting the reactor. 77,858.3 kg/hr of the products will flow from the transesterification reactor at 90°C and 50 bar into a decanter at 0°C and 1.38 bar. The decanter has been sized such that its residence time is approximately 10 minutes allowing for good separation between the two liquid phases that exit the reactor.

Following the residence time, two different streams are pumped out of the decanter. The glycerol rich stream, seen in Figure 12.2 as Stream 2, pumps 9,562kg/ hr of glycerol and methanol with very trace amounts of FAMEs from the decanter to a flash vessel. The flash vessel, run at 0.344 bar and 163.8 °C, separates the excess methanol from the free glycerol based on their differences in volatility. After their separation, the methanol comes off the top of the flash vessel (Stream 4) at a rate of 5,015 kg/hr and will be condensed and returned to the transesterification reactor from the initial portion of the process. The glycerol leaves the flash vessel (Stream 3) at a rate of 4,546 kg/hr and a purity of 99.5% glycerol by weight. It will be sent to storage containers and then sold to offset the price of the rest of the process.

The other stream from the decanter (Stream 5) is a FAMEs rich stream that also contains amounts of methanol and glycerol. It will be pumped from the decanter at a rate of 68,295 kg/hr into a flash vessel run at 235°C and 1 bar. The flash vessel separates the FAMEs from the excess methanol and is used because a distillation column showed little improvement in removing the residual glycerol from the stream and ran at a higher temperature. FAMEs decompose at approximately 300° C. Therefore, it is essential to keep the temperature significantly below this number. The methanol (Stream 6) is pumped out of the flash vessel at a rate of 1,745 kg/ hr and returned to the other half of the process where it will be condensed and reused in the transesterification reactor. The FAMEs product off the bottom of the flash vessel (Stream 7) is pumped out at a rate of 66,550 kg per hour. These FAMEs are now considered viable as product

biodiesel. Following the separation into the reactor, the FAMEs are pumped (Stream 8) to a splitter, seen in Figure 12.3 as P2-D, which separates the stream sending 11.5% of the FAMEs (Stream 10) to the methyl EPA/DHA separation process. The remaining 88.5% is split off (Stream 9) and pumped into storage tanks where it then will be sold as biodiesel.

Following the splitter, 7,625 kg/hr of FAMEs is pumped through a heat exchanger to reduce the temperature of the FAMEs to 35 ℃. 44,000 kg/hr of water flows counter-currently through the heat exchanger entering at 32.2 ℃ and exiting at 48.9 ℃. Once cooled, the FAMEs (Stream 11) is pumped to the first of two counter-current liquid-liquid extraction processes. LLE 1, seen as P2-F in Figure 12.3, is a countercurrent column that will flow the FAMEs from the bottom of the column and a 4M solution of silver nitrate in methanol from the top of the column. The silver nitrate mixture is made up of 4,250 kg of silver nitrate and 4,955 kg of methanol. It will be mixed in advance and after initial startup will be continuously recycled through the separation processes. The 7,625 kg/ hr of FAMEs will flow counter-currently against the 9,205 kg/hr of silver nitrate methanol mixture (Stream 13). The liquid contacting will cause the methyl EPA and methyl DHA to complex with the free silver ions in the silver methanol mixture and move into this phase, leaving the FAMEs. Because of the density difference, the remaining light FAMEs will be removed at the top of the column (Stream 14) at a rate of 6,185 kg/ hr. The light FAMEs will be pumped from the separation into storage tanks where they can be recombined with the other FAMEs and sold as biodiesel.

The other flow coming out of the bottom of the LLE (Stream 15) is a mixture of the methanol and silver complexed methyl Omega-3s. The stream flows from the bottom of the column at a rate of 10,645 kg/ hr. The flow will then be pumped up to the top of the second liquid-liquid extraction marked as P2-G in the flow diagram Figure 12.3. This mixture (Stream 16) will flow from the top of the column against 3,200 kg/ hr of 1- hexene (Stream 18). The 1-hexene acts as a stripping agent to uncomplex the methyl Omega-3s which then move into the 1-hexene. The silver methanol mixture is removed from the bottom of the column (Stream 19) at a rate of 9,204 kg/ hr and is recycled back to the first LLE process (Stream 20). A mixer and inlet stream (Stream 12) is accounted for in the flow diagram so that any possible loss of the mixture over time can be replaced with fresh mixture. This loss should not be a significant concern. The methyl EPA and methyl DHA in 1- hexene (Stream 21) come out of the top of the column at a rate of 4,641 kg/ hr. The stream then flows into a flash vessel (P2-H in Figure 12.3) at 107 ℃

and 0.133 bar. The flash vessel separates the methyl EPA/ DHA from the 1-hexene. The 1-hexene leaves the top of the column (Stream 22) at a rate of 3,184 kg/hr and is condensed using a heat exchanger. The heat exchanger flows 23,390 kg/hr of water counter-currently that enters at 32.2℃ and exits at 35.8 ℃. The condensed 1-hexene (Stream 23) is then pumped back to the second LLE column. Because the 1-hexene, methyl EPA DHA separation is not perfect, fresh 1-hexene must be added to the recycle stream to ensure that 3,200 kg/hr is being pumped to the column. Therefore, the recycles stream is pumped to a mixer where 16 kg/ hr is added (Stream 17) before it is sent back to the second LLE (Stream 18). The methyl EPA DHA is pumped out of the bottom of the column (Stream 25) at a rate of 1,456.83 kg/hr. There is still a small amount of 1-hexene in the stream making up approximately 1% by weight. However, since the EPA DHA will go through additional separations after their reaction and the 1-hexene will not hinder the reaction process, no additional separation was added at this step in the process.

Following the separation of the methyl Omega-3s from the rest of the FAMEs, the methyl esters are pumped at a rate of 1,440 kg/hr to a base-reactive section (P3-K), consisting of two stirred tank reactors in series (Stream 26). All the methyl ester stream will enter in the first reactor. Also sent into the first reactor are 870 kg/hr of methanol (Stream 35) which are recycled in from the distillation to follow and 1,030 kg/hr of aqueous NaOH solution (Stream 30). This NaOH solution is prepared in a storage tank (P3-J) which has inlets of 430 kg/hr of 50 wt% NaOH in water (Stream 27) along with 590 kg/hr of process water (Stream 28). The reactive section consists of two stirred tanks in series, with all material being pumped into the first tank. The material stays in this section for an overall residence time of 2 hours, with each tank having an individual residence time of 1 hour (the actual residence time of each tank due to equipment size constraints is 68 minutes). The tanks are maintained at 65°C by using external water jackets for removing excess heat (P3-KJ) and perform these reactions at near atmospheric pressures.

Exiting the reactive section is a single-phase liquid stream (Stream 31) composed of the carboxylate ions of EPA and DHA, methanol, and NaOH dissolved aqueous solution. The combined stream flows at a rate of 3,340 kg/hr and is pumped to a distillation column (P3-L) with 20 stages that operate at 125℃ and 1.5-1.8 bar throughout the tower with a molar reflux ratio of 0.85. Coming out of the tower is a distillate stream (Stream 33) with a flow rate of 1,010 kg/hr that is 99.5 mol% methanol, and a bottoms stream (Stream 37) with a flow rate of 2,330 kg/hr. The distillate stream passes through a splitter where approximately 870 kg/hr gets recycled

to the base-reactive section (Stream 34) after passing through a heat exchanger, and the remainder (Stream 36) are sent to the triglyceride transesterification reactor. The heat exchanger (P3-N) uses 1,870 kg/hr of cooling water to cool the 870 kg/hr of methanol from 74.9°C to 35°C.

The bottoms stream of the distillation column containing fatty acid carboxylates, with residual methanol, NaOH, and water leave at a rate of 2,330 kg/hr. This mixture (Stream 37) is then sent to the acid-reactive section of the process (P3-P), containing two more stirred tank reactors in series with an overall residence time of 1 hour. Stream 37 and 870 kg/hr of aqueous HCl solution (Stream 41) are sent into the first of the two stirred tanks in P3-P. The aqueous HCl solution is prepared in a storage tank (P3-O) with inlets of 710 kg/hr of 30 wt% HCl in water (Stream 38) and 160 kg/hr of water (Stream 39). Each stirred tank has a residence time of at least 30 minutes (the actual residence time due to equipment size constraints is 36 minutes) and operates at 1.2 bar and 25°C. Each stirred tank is enclosed in a jacket filled with chilled water (P3-PJ) to provide the heat transfer necessary for maintaining the low desired reaction temperature. The resultant mixture (Stream 42) after the reaction goes to completion should exist in two liquid phases.

The first liquid phase is a lighter, oily phase containing 1375 kg/hr of EPA and DHA, now in their carboxylic acid form. The second liquid phase is a heavier, aqueous phase containing 5 kg/hr of methanol, 320 kg/hr of NaCl, and 15 kg/hr of HCl completely solvated in 1,480 kg/hr of process water. This two-phase liquid stream (Stream 42), with a total flow rate of 3,200 kg/hr, is sent into a decanter (P3-Q). The decanter is used to separate the oily EPA and DHA from the aqueous components and is designed to have a length-to-diameter ratio of 4 and a residence time of approximately 40 minutes. Both streams leaving the decanter are then sent to storage tanks with a capacity to hold them for seven days. As a wastewater pre-treatment step, the aqueous components are neutralized in the aqueous storage tank (P3-S) by adding a stoichiometric amount of NaOH relative to HCl. The acid-base chemistry within P3-S results in a small temperature increase of about 5°C.

14. Energy Balance and Utility Requirements

Several processes in this plant will require heating or cooling. The reasoning for why each component may require a transfer of energy is described in Section 10 but can be generalized to being used for attaining the required conditions for a separation or a reaction. The items which do require some transfer of energy are listed in Table 14.1, which lists the items along with the magnitude of energy transfer required. Positive heat duties correlate to items which requiring heating and negative heat duties correlate to items which require cooling.

Table 14.1 Energy Demands of Equipment

Equipment ID	Equipment Description	Heat Duty (kW)
P1-A	FAME-Glycerol-Methanol Decanter	-4,878
P1-B	Glycerol-Methanol Flash Vessel	+2,596
P1-C	FAME-Methanol Flash Vessel	+10,341
P2-E	FAME Cooler	-981
P2-H	FAME-Hexene Flash Vessel	+520
P2-I	Hexene Condenser	-112
P3-KJ	NaOH Reactor Water Jacket	-37
P3-LC	Omega-3-Methanol Distillation Condenser	-562
P3-LR	Omega-3-Methanol Distillation Reboiler	+668
P3-N	Methanol Cooler	+35
P3-PJ	HCl Reactor Water Jacket	-177

As a result of having to meet the various heat duties listed in Table 14.1, several utilities need to be bought for heating and cooling the materials in this process. In general, these temperature maintenance utilities are water, except the refrigerant which is probably some natural gas. Table 14.2 lists the energy demands and costs of purchasing the temperature maintenance utilities, with prices referenced from Seider (Seider et al., 2017, p. 500).

Table 14.2 Quantities and Costs of Cooling and Heating Utilities Required

Utility	Equipment ID	Quantity	Quantity	Annual Cost
		(GJ/hr)	**(GJ/yr)**	**($/yr)**
Natural Gas Refrigeration ($6.47/GJ)	P1-A	17.56	138,443.04	895,726.47
	Total	**17.56**	**138,443.04**	**895,726.47**
		(tons)	**(ton-day)**	**($/yr)**
Chilled Water ($1.50/ton-day)	P3-PJ	50.23	16501.62	24752.43
	Total	**50.23**	**16501.62**	**24752.43**
		(gal/hr)	**(gal/yr)**	**($/yr)**
Cooling Water ($0.10/1000 gal)	P2-E	6178.980	48931589.78	4893.16
	P2-I	11623.570	92047515.77	9204.75
	P3-KJ	506.48	3993127.36	16.71
	P3-LC	11493.00	90610812.00	379.27
	P3-N	494.94	3902124.23	16.33
	Total	**30296.97**	**239485169.14**	**14510.22**
		(lb/hr)	**(lb/yr)**	**($/yr)**
High Pressure Steam (450 psig) ($8.00/1000 lbs)	P1-B	47736.707	378028894.57	3024231.16
	P1-C	11985.600	94914445.82	759315.57
	P2-H	1089.350	8626606.22	69012.85
	P3-LR	2566.08	20230966.84	161847.73
	Total	**63377.737**	**501800913.45**	**4014407.31**

In addition to the utilities needed for energy transfer, the plant will also require electricity to power the pumps required by this process. Many of the flows in this process operate close to room temperature and will require a pressure differential to enable materials to flow through the process. Table 14.3 lists the electrical demands of the pumps that are installed in the process as well as the annual cost of purchasing the required energy. Referencing Seider, a price of $0.07/kW-hr was selected as the price of electricity to be purchased from a utility.

Table 14.3 Quantities and Costs of Electricity Required by Pumps

Equipment ID	Quantity (kW-hr)	Quantity (kW-yr)	Annual Cost ($/yr)
P1-CP	0.711	5630.44	394.13
P2-FP	0.069	546.41	38.25
P2-GP	0.063	498.90	34.92
P2-HP	0.121	961.28	67.29
P2-IP	0.030	237.57	16.63
P3-JP	0.0159	125.44	8.78
P3-KP	0.3006	2369.96	165.90
P3-LP	0.2231	1758.77	123.11
P3-OP	0.0431	339.83	23.79
Total	**1.5767**	**12468.6**	**872.80**

Dilution of the strong acid and base used in this process will be required for reasons described in Section 10.4. Process water will need to be purchased for diluting these compounds. Additionally, the wastewater emerging from the process will have some residual organic compounds which may require additional treatment. Both items will be considered as utilities in this process and will be purchased for the prices listed in Seider. The amounts of costs of these quantities are listed in Table 14.4.

Table 14.4 Other Utilities

Utility	Equipment ID	Quantity	Quantity	Annual Cost
		(gal/hr)	**(gal/yr)**	**($/yr)**
Process Water ($0.80/1000 gal)	P3-J	157.21	1239441.79	991.55
	P3-O	41.73	328965.45	263.17
	Total	**198.94**	**1568407.24**	**1254.73**
		(lb/hr)	**(lb/yr)**	**($/yr)**
Wastewater Treatment ($0.15/lb organic)	P3-S	11.41	89991.23	13498.68
	Total	**11.41**	**89991.23**	**13498.68**

15. Equipment List and Unit Descriptions

15.1 Pressure Vessels

Transesterification Product (FAME-Glycerol-Methanol) Decanter

Unit ID: P1-A	Temperature: 0 ℃
Type: Decanter	Pressure: 1.38 bar
Material: Carbon Steel	Diameter: 6 ft
Specification Sheet: Section 16.1	Height: 17.5 ft
Costing Data: Section 18	Design Calculation: Section 25.4.1

The function of the decanter is to separate the two liquid phases the separate the transesterification reactor. 77,858 kg/hr of liquid will flow from the reactor at 90 ℃ and 50 bar into the decanter which operates at 1.38 bar and 0℃. The decanter will be made of carbon steel and will have a diameter of 6 ft and a height of 17.5 ft. The vessel was sized based on having an optimal residence time for the vessel between 5 to 10 minutes for good separation of the liquid phases. This vessel has a residence time of approximately 9.5 minutes. Because of the large change in temperature between the inlet stream and the unit temperature, this vessel requires a large amount of refrigeration. The low temperature decreases the amount of glycerol in the FAMEs heavy outlet stream. The heat duty required for this vessel is -4878 kWh which is satisfied using 17.6 GJ/ hr of refrigerant capable of cooling below 0℃.

Glycerol-Methanol Flash Vessel

Unit ID: P1-B	Temperature: 163.8 ℃
Type: Flash Vessel	Pressure: 0.345 bar
Material: Carbon Steel	Diameter: 3.5 ft
Specification Sheet: Section 16.1	Height: 12 ft
Costing Data: Section 18	Design Calculation: Section 25.4.1

The purpose of this flash vessel is to remove the excess methanol from the glycerol stream that exits the decanter. The important goal for this vessel was to reach at least 99.5% purity by weight glycerol as this is the market standard. In order to reach this requirement, the vessel runs at 163.8 ℃ and 0.345 bar. P1-B is a vacuum vessel, and therefore the pressure had to be taken into account when calculating the thickness of the vessel. Although it is a vacuum vessel, the minimum thickness for a vessel that is 12 ft tall was more than sufficient for the

minor vacuum produced in the vessel (Seider et al., 2017, p. 466). The heavy glycerol stream flows into the flash vessel at a rate of 9,562.4 kg/hr. The flash is 3.5 ft in diameter and 12 ft tall. The vessel was sized in Aspen Plus, and the sizing was checked to ensure that there was a residence time between 5 to 10 minutes in the vessel. The glycerol separation requires a heat duty of 2596.45 kWh which is satisfied by high-pressure steam at 450 psig at a rate of 11,985.6 lb/hr.

FAME-Methanol Flash Vessel

Unit ID: P1-C	Temperature: 235.4℃
Type: Flash Vessel	Pressure: 1 bar
Material: Carbon Steel	Diameter: 6 ft
Specification Sheet: Section 16.1	Height: 18 ft
Costing Data: Section 18	Design Calculation: Section 25.4.1

The purpose of this flash vessel is to remove the excess methanol and glycerol from the FAMEs heavy stream exiting the decanter. The requirements for biodiesel demand a maximum amount of free glycerol as 0.02% by weight of biodiesel product and the maximum amount of methanol as 0.2% by weight of biodiesel product. In order to get as close to these requirements as possible in the FAMEs product stream, the flash vessel is run at 235.4℃ and 1 bar. The FAMEs stream flows into the vessel at a rate of 68,295.9 kg/hr. The methanol exits out of the top of the vessel at a rate of 1,745.6 kg/hr and the FAMEs leave out of the bottom the vessel at a rate of 66,550.4 kg/hr. The flash vessel is 6 ft in diameter and 18 ft tall. It is sized to attain a residence time between 5 to 10 minutes. The FAMEs flash vessel requires an inlet net duty of 10,341.3 kWh which is satisfied with high-pressure steam at 450 psig flowing at 47,736.7 lb/hr.

FAME-Hexene Flash Vessel

Unit ID: P2-H	Temperature:106.9 ℃
Type: Flash Vessel	Pressure: 0.133 bar
Material: Carbon Steel	Diameter: 3 ft
Specification Sheet: Section 16.1	Height: 12 ft
Costing Data: Section 17	Design Calculation: Section 25.4.2

The purpose of this flash vessel is to separate the 1-hexene from the methyl Omega-3s after the LLE columns. Hexene is an impurity and may hinder optimal reaction and sale of

Omega-3s. A flash vessel running at 106.9 ℃ and 0.133 bar is capable of attaining the desired separation of this impurity from the methyl Omega-3s. This is a vacuum vessel, and therefore the pressure had to be taken into account when calculating the thickness of the vessel. The low pressure of 0.133 bar was used upon recommendation of the consultants who advised this project and provided information about typical pressures used for vacuum vessels in industry.

Additionally, the minimum thickness for a vessel of 12 ft tall as recommended by Seider was more than enough for the minor vacuum produced in the vessel (Seider et al., 2017, p. 466). The mixed stream flows into the flash vessel at a rate of 4,640.9 kg/hr. The flash is 3.5 ft in diameter and 12 ft tall. The vessel was sized in Aspen Plus, and the sizing was checked to ensure that there was a residence time between 5 to 10 minutes in the vessel. The FAME-hexene separation requires a heat duty of 520.264 kWh which is satisfied by high-pressure steam at 450 psig at a rate of 1,089.35 lb/hr.

NaOH Stirred Tank Reactor

Unit ID: P3-K	Temperature: up to 134.9℃
Type: Pressure Vessel	Pressure: up to 2.43 barg
Material: 304-Stainless Steel	Diameter: 4 ft
Specification Sheet: Section 16.1	Height: 13 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

After separation of Omega-3 FAMEs from other FAMEs, a hydrolysis reaction is required to obtain the final Omega-3 fatty acid product. The first step of the ester hydrolysis is a base-promoted step: by adding NaOH to the FAMEs, the fatty acid carboxylate and methanol are formed. Since NaOH is a corrosive material, the vessel is made of stainless steel to minimize the effects of corrosion and is designed with a corrosion thickness of at least 0.25 in, as recommended by Seider (Seider et al., 2017, p. 466). The reaction conditions are atmospheric pressure and 65°C, and the vessels are designed to accommodate those conditions. Each reactor has a volume of 4625 L. This was chosen since there is approximately 4100 L/hr of material entering and leaving the reactor and a residence time of 2 hours was chosen for this step. Since the desired fatty acid product will be formed in a step soon to come and is prone to oxidation in air, this vessel will need to be filled with an inert gas like nitrogen.

Additionally, two vessels are required and are placed in series, to optimize the likelihood that material will stay within this stage for the desired residence time. The vessel will require 37

kWh of cooling, to be provided by cooling water flowing through P3-KJ. 1440 kg/hr of FAMEs at 107℃, 1030 kg/hr of NaOH at 55℃ (aq), and 870 kg/hr of methanol at 35℃ enter the first vessel in P3-K, and 3340 kg/hr of material (i.e., fatty acid carboxylates, methanol, residual NaOH) at 65℃ exit the second vessel. An agitator will need to be purchased to ensure sufficient mixing of reactants in these vessels.

HCl Stirred Tank Reactor

Unit ID: P3-P	Temperature: up to 155.3℃
Type: Pressure Vessel	Pressure: up to 2.43 barg
Material: 304-Stainless Steel	Diameter: 3 ft
Specification Sheet: Section 16.1	Height: 10 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

P3-P is responsible for conducting the acid-promoted step of the FAME hydrolysis. In this second step, HCl will react with the fatty acid carboxylate to form the desired Omega-3 fatty acid and water. The vessel is again made of stainless steel to minimize the corrosive effects of HCl on the vessel's durability and longevity. The reaction conditions are slightly above atmospheric pressure and 25°C, and the vessels are designed to maintain these conditions. Additionally, each vessel has a residence time of 30 minutes and can hold a volume of 2000 L, which is appropriate as the volume exiting these reactors will be about 3300 L/hr. The remaining volume of the reactors will need to be filled with inert gas since the fatty acids are susceptible to oxidation in air. Again, two vessels are required and will be placed in series to optimize the likelihood that material will stay within this stage for the desired residence time. 2330 kg/hr of aqueous fatty acid carboxylate at 127℃ and 870 kg/hr of HCl (aq) at 37℃ enter P3-P, and 3200 kg/hr of fatty acid-aqueous solution exit at 25℃. A heat duty of 177 kWh will need to be removed to attain the stated exit temperature and is achieved by using a jacket with chilled water (P3-PJ). An agitator will also need to be purchased to ensure enough mixing of reactants.

Omega-3-Water Decanter

Unit ID: P3-Q	Temperature: up to 121.1℃
Type: Pressure Vessel	Pressure: up to 2.43 barg
Material: 304-Stainless Steel	Diameter: 3 ft
Specification Sheet: Section 16.1	Height: 12 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

Coming out of reactors P3-P is a 3200 kg/hr liquid stream which is predicted to be two immiscible phases. One of these phases consists of the desired Omega-3 fatty acids; the other phase consists of methanol, water, and some ionic species from the dissociation of strong acids and bases used previously. The decanter was calculated by Aspen Plus to have a volume of 2400 L, which will hold more than the desired residence time of 30 minutes. This greater residence time is advantageous since the density differences between the two phases is relatively small, and greater time within the reactor should allow for the ideal separation which was modeled. Since some residual HCl from the prior step still exists, the decanter will need to be made of stainless steel. Exiting this decanter are 1375 kg/hr of Omega-3 fatty acids which will be sent to P3-Q and 1825 kg/hr of wastewater which will be sent to P3-R. All streams entering and leaving P3-Q are at 25℃ and approximately atmospheric pressure.

15.2 Columns

FAME-Silver Liquid-Liquid Extraction

Unit ID: P2-F	Temperature: 35℃
Type: Tray Column	Pressure: 1 bar
Material: Carbon Steel	Diameter: 6 ft
Specification Sheet: Section 16.2	Height: 12.5 ft
Costing Data: Section 17	Design Calculation: Section 25.2

The purpose of P2-F is to extract the methyl Omega-3s from the inlet FAMEs stream. This extraction can be performed in a column by flowing the less dense FAMEs from the bottom of the column and a denser 4M solution of silver nitrate in methanol from the top of the column. The silver nitrate mixture is made up of 4,250 kg of silver nitrate and 4,955 kg of methanol. It will be mixed in advance and after initial startup will be continuously recycled through the separation processes. The 7,625 kg/hr of FAMEs will flow counter-currently against the 9,205 kg/hr of silver nitrate methanol mixture.

FAME-Hexene Liquid-Liquid Extraction

Unit ID: P2-G	Temperature: 35℃
Type: Tray Column	Pressure: 35℃
Material: Carbon Steel	Diameter: 4 ft
Specification Sheet: Section 16.2	Height: 10 ft
Costing Data: Section 17	Design Calculation: Section 25.2

The purpose of P2-G is to strip the Omega-3s from the silver nitrate methanol mixture and extract them into the 1-hexene solvent phase. The silver methanol mixture is removed from the bottom of the second column at a rate of 9,204 kg/hr and is recycled back to P2-F. A mixer and inlet stream for silver nitrate are accounted for in the flow diagram (Section 12.3) so that any possible loss of the mixture over time can be replaced with fresh mixture. This is not expected to be necessary as Teramoto paper found that loss of the silver ions was negligible and there was little to no miscibility between streams (Teramoto, 1994). However, Teramoto's work was performed at lab scale, and small losses at that scale may be significant at an industrial scale. Therefore it was decided to have an inlet stream accounted for in case there is a quantifiable loss of the silver nitrate over time. The methyl EPA and DHA in 1-hexene come out of the top of the column at a rate of 4,641 kg/hr.

When designing these pieces of equipment, the calculations were based on removing 99% of the EPA and DHA from the inlet FAMEs, and that the stripping agent (4M silver nitrate) would be 88% effective. Both of these values were calculated from partition coefficients and efficiencies from the literature and were used to estimate the flow rates entering and leaving these extraction columns (Teramoto, 1994; Li 2009). Applying the partition coefficient and the calculated flow rates, the Kremser equation was then used to determine the total number of theoretical trays in each of the columns. Because there was little data available on the efficiency of this process, it was suggested by the project's consultants to assume a fairly low efficiency. Therefore, the total number of trays in the columns was determined by setting the efficiency to 25%.

Because there was no data available about the mass transfer variables for both of the LLEs it was difficult to model the internals of the columns. Therefore, when it came to sizing the industrial columns, the decision was made to size them based on optimal residence time for the extractions. This was determined from a paper by Li that found that the optimal residence time for the complexation of silver ions and methyl Omega-3s was approximately 25 minutes (Li, 2009). It was found that any more time in the column would not increase the amount of methyl Omega-3s produced. For the second column, 5 to 10 minutes was more than a sufficient amount of time for the 1-hexene to strip the methyl Omega-3s from the silver solution. The columns were sized and priced like distillation tray columns as they are similar in materials and internals. From this sizing, it was found that P2-F is 6 ft in diameter and 12 ft tall with 9 trays and that P2-G is 4 ft in diameter and 10 ft tall with 20 trays. The smaller size of P2-G reflects the shorter residence time. If this plant were to be built, it would be essential that a pilot scale LLE process is tested to have quantitative data to determine the actual efficiencies of the column, as well as the mass transfer variables and other internals necessary to size the columns more vigorously.

Omega-3-Methanol Distillation Column

Unit ID: P3-L	Temperature: up to 154°C
Type: Distillation Column	Pressure: up to 2.42 barg
Material: 304-Stainless Steel	Diameter: 2.5 ft
Specification Sheet: Section 16.2	Height: 52 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

The reaction of FAME with NaOH also produces a stoichiometric equivalent of methanol as a byproduct. Methanol serves as both a solvent for the reaction mentioned before and as a reactant in the transesterification reactor in Yadav's process (out of scope). Thus, the distillation column serves to return some of the methanol that solvated the NaOH-promoted reaction and reduces the amount of methanol that needs to be purchased for the transesterification of triglycerides. In effect, this column serves to reduce the cost of associated with purchasing methanol, with the added benefit of reducing the volume of the entering stream. This allows subsequent reactors to be built to accommodate a smaller volume.

The inlet of the distillation tower is a stream containing 3340 kg/hr of material that was pumped from P3-KP. Exiting the tower is a 1010 kg/hr distillate that is 99.5 mol% methanol, and the remaining 2330 kg/hr bottoms. This separation was calculated by Aspen Plus to require 20 stages, with the feed entering at stage 11. Each stage will be 2 ft apart, and the diameter of the column was calculated to be 2.5 ft. This diameter is rather narrow for a distillation column, and one of the project authors (Fabiano) noted that cartridge trays would be necessary. The condenser associated with the tower requires 43500 kg/hr of cooling water which will be heated from 90°F to 120°F to cool 560 kWh of heat duty, and the reboiler will be heated using 1160 kg/hr of steam at 100 psi to provide 670 kWh of heat duty. The molar reflux ratio associated with the tower is 0.85.

15.3 Heat Exchangers

FAME Cooler

Unit ID: P2-E	Inlet Temperature: 235℃
Type: Shell and Tube Heat Exchanger	Outlet Temperature: 35℃
Material: Carbon Steel	Cooling Water Amount: 44,000kg/hr
Specification Sheet: Section 16.3	Surface Area: 344.5 ft^2
Costing Data: Section 17	Design Calculation: Section 25.4.1

The purpose of this heat exchanger is to reduce the temperature of the FAMEs stream to 35 ℃ before it enters the LLE process. Because solubility is dependent on temperature, and the available data for LLE processes was in the range of 35℃ it was essential for the proper extraction of the methyl Omega-3s that the LLEs occur at the correct temperature. Therefore, a heat exchanger was added. The heat exchanger is carbon steel and has a surface area of 344.5 ft^2. P2-E reduces the temperature of the FAMEs from 235℃ to 35 ℃. In order to reduce the temperature this far, the heat exchanger requires 44,000 kg/hr of cooling water which enters at 32.2 ℃ and exits at 48.9 ℃. The heat exchanger was modeled and priced as a fixed head, 1-1 shell and tube heat exchanger. The heat exchanger has a net heat duty of 981 kWh which is satisfied by the heat transfer between the FAMEs stream and the cooling water.

1-Hexene Condenser

Unit ID: P2-I	Inlet Temperature: 106.9℃
Type: Shell and Tube Heat Exchanger	Outlet Temperature: 35℃
Material: Carbon Steel	Cooling Water Amount: 23390 kg/hr
Specification Sheet: Section 16.3	Surface Area: 67.56 ft^2
Costing Data: Section 17	Design Calculation: Section 25.4.2

The purpose of this heat exchanger is to condense the 1- hexene that flows out of the top of the flash vessel. The 1-hexene leaves the top of the column and enters the heat exchanger at a rate of 3,184 kg/hr. The heat exchanger flows 23,390 kg/hr of water counter currently that enters at 32.2℃ and exits at 35.8 ℃. The heat exchanger is carbon steel and has a surface area of 67.56 ft^2. It reduces the temperature of the 1-hexene from 106.9℃ to 35 ℃. The heat exchanger was modeled and priced as a fixed head, 1-1 shell and tube heat exchanger. The heat exchanger has a net heat duty of 112.4 kWh which is satisfied by the heat transfer between the 1-hexene and the cooling water.

NaOH Reactor Water Jacket

Unit ID: P3-KJ	Temperature: up to 134.9℃
Type: Pressure Vessel	Pressure: up to 2.43 barg
Material: Carbon Steel	Diameter: 4.5 ft
Specification Sheet: Section 16.1	Height: 13.5 ft
Costing Data: Section 17	Design Calculation: Section 25.2

Since the FAME inlet stream enters at a temperature above the reaction conditions, some cooling is needed. From modeling this reactor in Aspen Plus, a heat duty of 37 kWh needs to be removed from P3-K. Since there is enough surface area from the size of vessels P3-J, larger vessels can be built to encapsulate the vessels carrying out the reaction and contain cooling water to provide the necessary heat transfer for maintaining heat conditions. These larger vessels, or jackets, are sized to be slightly larger than the vessels they are trying to cool and can be crafted with carbon steel since there is only water in it. P3-KJ will have 1920 kg/hr of cooling water flowing through the space between the walls of P3-KJ and P3-K to provide enough heat transfer while keeping the temperature of the cooling water low enough to prevent mineral deposition. The cooling water enters at 32℃ and exits at 49℃.

Omega-3-Methanol Distillation Column Condenser

Unit ID: P3-LC	Temperature: up to 121.1℃
Type: Shell and Tube Heat Exchanger	Pressure: up to 2.43 barg
Material: Carbon Steel	Cooling Water Amount: 43,505 kg/hr
Specification Sheet: Section 16.3	Surface Area: 160.58 ft^2
Costing Data: Section 17	Design Calculation: Section 25.4.3

P3-LC is part of distillation column P3-L and is responsible for condensing the material that vaporizes from the column to its bubble point. 43,505 kg/hr was the amount of cooling water calculated by Aspen Plus to remove 560 kWh of heat duty using a 1-shell, 1-pass heat exchanger. P3-LC was also sized by Aspen to provide enough surface area for heat transfer. Minimal amounts of NaOH are predicted to vaporize, so the cheaper carbon steel was selected as the material of construction. The material leaves the condenser at 75℃.

Omega-3-Methanol Distillation Column Reboiler

Unit ID: P3-LR	Temperature: up to 192℃
Type: U-Tube Heat Exchanger	Pressure: up to 7.6 barg
Material: 304-Stainless Steel	Steam Amount: 1,163.95 kg/hr
Specification Sheet: N/A	Surface Area: 288.38 ft^2
Costing Data: Section 17	Design Calculation: Section 25.4.3

P3-LR is part of distillation tower P3-L and is responsible for boiling-up the material that leaves from the bottom of the column. 1,163.95 kg/hr was the amount of steam calculated by Aspen Plus to provide 670 kWh of heat duty. P3-LR was also sized by Aspen as a U-tube heat exchanger to provide enough surface area for heat transfer. Almost all the NaOH entering the distillation column is expected to pass through the reboiler, demanding the use of stainless steel as the material of construction. 2330 kg/hr of non-boiled up material leaves the reboiler at 127℃. P3-LR has a molar boil-up ratio of 1.036.

Methanol Cooler

Unit ID: P3-N	Temperature: up to 121.1℃
Type: Shell and Tube Heat Exchanger	Pressure: up to 2.43 barg
Material: Carbon Steel	Cooling Water Amount: 1,873.56 kg/hr
Specification Sheet: Section 16.3	Surface Area: 43.62 ft^2
Costing Data: Section 17	Design Calculation: Section 25.4.3

If the material from splitter P3-M (which receives material from the distillate of P3-L) were immediately recycled back to the NaOH-reactors P3-K, more cooling would be required. The water jacket solution the process currently uses would not be able to provide enough cooling, and a more expensive option would need to be applied to that step. Since that reactor also contains corrosive NaOH, that heat exchanger would need to be made of stainless steel. Additionally, since there are multiple reactor vessels, there might be multiple heat exchangers in place. A simple way to avoid this would be to simply cool the methanol stream before recycle – Aspen calculated that the 1-shell, 1-tube heat exchanger to perform this cooling would need 1,873.56 kg/hr of cooling water to remove 35 kWh of heat duty over a surface area of 43.62 ft^2.

HCl Reactor Water Jacket

Unit ID: P3-PJ	Temperature: up to 155.3℃
Type: Pressure Vessel	Pressure: up to 2.43 barg
Material: Carbon Steel	Diameter: 3.5 ft
Specification Sheet: Section 16.1	Height: 10.5 ft
Costing Data: Section 17	Design Calculation: Section 25.2

Similar to how P3-KJ provides the heat transfer for P3-K, P3-PJ describes the water jackets which will provide the requisite heat transfer for P3-P. 6080 kg/hr of chilled water will run through the jackets from 7℃ to 32℃ to remove 177 kWh from P3-P.

15.4 Pumps

The majority of the pumps for this process were not modeled in great detail. Because the purpose of these pumps is simply to continue the flow of the streams between vessels, the pumps were designed to ensure that enough power was available for flow and that is all. Therefore, based off the suggestion of this design's consultants, all of the pumps have 50 ft of available head and create a difference in pressure of approximately 2-3 psia in order to continue the flow of the streams in the process. Variances in the energy requirements are a result of the varying size and density of the flows being pumped through each piece of equipment. The total energy requirements for the pumps in this process is 1.5767 kW-hr, and it is fulfilled with purchased electricity. The composition, flow rate, and temperature of material entering a given pump is the same as that leaving the said pump. All the pumps used in this design are centrifugal pumps with a shaft rpm of 3,600 and a VSC orientation.

P1-CP is used within the Separation of Transesterification Reactor Products portion of the design (Section 12.2).

FAMEs Pump to Splitter P2-D

Unit ID: P1-CP	Temperature: 235.4℃
Type: Centrifugal Pump	Pressure Change: 0.2 bar
Material: Carbon Steel	Energy Requirement: 0.711 kWh
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.4.1

The following pumps are used within the Separation of Omega-3 Methyl Esters from FAME Mixture portion of the design (Section 12.3).

FAME-Silver Pump

Unit ID: P2-FP	Temperature: 35℃
Type: Centrifugal Pump	Pressure Change: 0.1 bar
Material: Carbon Steel	Energy Requirement: 0.069 kWh
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.4.1

Silver Nitrate Recycle Pump

Unit ID: P2-GP	Temperature: 35℃
Type: Centrifugal Pump	Pressure Change: 0.1 bar
Material: Carbon Steel	Energy Requirement: 0.063 kWh
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.4.1

Methyl Omega-3 Pump from Flash Vessel to Base Reaction

Unit ID: P2-HP	Temperature: 106.9℃
Type: Centrifugal Pump	Pressure Change: 1.067 bar
Material: Carbon Steel	Energy Requirement: 0.1213 kWh
Specification Sheet: Section 16.4	Head: 30.06 ft
Costing Data: Section 17	Design Calculation: Section 25.4.1

1-Hexene Recycle Pump

Unit ID: P2-IP	Temperature: 35℃
Type: Centrifugal Pump	Pressure Change: 0.1 bar
Material: Carbon Steel	Energy Requirement: 0.0304 kWh
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.4.1

The following pumps are utilized within the Hydrolysis of FAMEs to Free Fatty Acids portion of this process (Section 12.4). Except for P3-LC, which is exposed to minimal acid and base, all of the pumps below are constructed with stainless steel to pump the corrosive material (strong acid or strong base) which passes through them.

NaOH Tank Pump

Unit ID: P3-JP	Temperature: 25℃
Type: Centrifugal Pump	Pressure Change: 0.2 bar
Material: 304-Stainless Steel	Energy Requirement: 0.016 kW
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

NaOH Reactor P3-K to Distillation Column P3-L Pump

Unit ID: P3-KP	Temperature: 65℃
Type: Centrifugal Pump	Pressure Change: 0.8 bar
Material: 304-Stainless Steel	Energy Requirement: 0.301 kW
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.2

Omega-3-Methanol Distillation Column Reflux Pump

Unit ID: P3-LP	Temperature: 74.9℃
Type: Centrifugal Pump	Pressure Change: 0.5 bar
Material: Carbon Steel	Energy Requirement: 0.223 kW
Specification Sheet: Section 16.4	Head: 100 ft
Costing Data: Section 17	Design Calculation: Section 25.2

HCl Tank Pump

Unit ID: P3-OP	Temperature: 25℃
Type: Centrifugal Pump	Pressure Change: 0.4 bar
Material: 304-Stainless Steel	Energy Requirement: 0.043 kW
Specification Sheet: Section 16.4	Head: 50 ft
Costing Data: Section 17	Design Calculation: Section 25.2

15.5 Storage Tanks

NaOH Storage Tank

Unit ID: P3-J	Temperature: 25°C
Type: Storage Tank	Pressure: 1.01 bar
Material: 304-Stainless Steel	Type: Cone roof
Specification Sheet: Section 16.5	Volume: 8,053 gal
Costing Data: Section 17	Design Calculation: Section 25.2

The preparation of NaOH with the desired amount of water for this process requires the mixing of aqueous NaOH and process water. Adding water to a base is known to be exothermic. However, there are already restrictions on how much heat can be removed from the base reactors P3-K due to the choice of water jackets to cool the entering FAMEs. Preparation of the aqueous NaOH in a separate tank would allow the heat formed to dissipate, making this exothermic behavior a non-issue. This tank is sized to hold the equivalent of a day's worth of NaOH demanded by the process and is made of stainless steel to account for the corrosive behavior of NaOH. P3-J combines 434 kg/hr of 50 wt% NaOH in water with 595 kg/hr of water to create an exiting stream of 1030 kg/hr of a diluted NaOH (aq) solution.

Omega-3-Methanol Distillation Column Reflux Accumulator

Unit ID: P3-LD	Temperature: up to 121.1℃
Type: Reflux Accumulator	Pressure: up to 2.43 barg
Material: Carbon Steel	Diameter: 3 ft
Specification Sheet: N/A	Height: 9 ft
Costing Data: Section 17	Design Calculation: Section 25.4.3

P3-LD is the reflux accumulator associated with distillation column P3-L for accumulating the distillate coming from condenser P3-LC before either returning the fluid to the column (reflux) or sending it out of the distillation tower (distillate). Aspen calculated the requisite sizing for this vessel. 1880 kg/hr of 99.5% methanol at 75℃ enters and leaves this accumulator.

HCl Storage Tank

Unit ID: P3-O	Temperature: 25℃
Type: Storage Tank	Pressure: 1.01 bar
Material: 304-Stainless Steel	Type: Cone roof
Specification Sheet: Section 16.5	Volume: 7,436 gal
Costing Data: Section 17	Design Calculation: Section 25.2

Similar to the motivation behind P3-J, preparing aqueous HCl by adding water to relatively concentrated HCl is also exothermic. The restriction of heat that can be removed easily by the water jackets is again present, and so preparation of the acidic solution in a separate vessel is advantageous. This tank is sized to hold the equivalent of a day's worth of HCl demanded by the process and is made of stainless steel to account for the corrosive behavior of HCl. 714 kg/hr of 30 wt% HCl in water and 158 kg/hr of water enter P3-O, and 872 kg/hr of dilute HCl (aq) exits P3-O.

Omega-3 Storage Tank

Unit ID: P3-R	Temperature: 25℃
Type: Storage Tank	Pressure: 1.2 bar
Material: 304-Stainless Steel	Type: Cone roof
Specification Sheet: Section 16.5	Volume: 111,157 gal
Costing Data: Section 17	Design Calculation: Section 25.2

The 1375 kg/hr of Omega-3 fatty acids that this design produces needs to be stored for some time before it can be shipped to another company for processing. P3-R is designed to hold the material for 7 days: this short length of time was chosen due to how prone the Omega-3s are to oxidation. This storage tank will also need to be kept slightly pressurized and filled with nitrogen as a precaution against oxidation in air. A third precaution to prevent oxidation is to manufacture the vessel from stainless steel.

Water Neutralization/Storage Tank

Unit ID: P3-S	Temperature: 25℃
Type: Storage Tank	Pressure: 1.2 bar
Material: 304-Stainless Steel	Type: Cone roof
Specification Sheet: Section 16.5	Volume: 109,456 gal
Costing Data: Section 17	Design Calculation: Section 25.2

P3-S stores the wastewater emerging from decanter P3-Q and acts as a place for pH pre-treatment. The 1824 kg/hr of slightly acidic wastewater from P3-Q needs to be neutralized with a base, as mentioned in Section 10.4. This neutralization is accomplished by adding 36 kg/hr of 50 wt% NaOH in water. The addition of base to acid is slightly exothermic, but Aspen predicts the rise in temperature to be slightly above room temperature (29.6°C). The presence of the strong base with the acid necessitates the use of stainless steel as the material of construction.

16. Specification Sheets

16.1 Pressure Vessels

Transesterification Product (FAME-Glycerol-Methanol) Decanter

Identification: Item: Horizontal Pressure Vessel; Item No.: P1-A; No. Required: 1

Function: Separate products in stream from transesterification reactor

Operation: Continuous

Materials Handled:

	Feed	Liquid 1	Liquid 2
Temperature (°C)	90	0	0
Pressure (bar)	50	1.38	1.38
Component mass flow (kg/hr)			
C14:0-ME	4178.3	4178.3	0
C16:0-ME	20461.3	20461.3	0
C16:1-ME	10909.9	10909.9	0
C18:0-ME	1493.1	1493.1	0
C18:1-ME	10295.1	10295.1	0
C18:2-ME	5436.8	5436.8	0
EPA-ME	13415.2	13415.2	0
DHA-ME	912.4	912.4	0
Methanol	5493.3	1174.11	4319.2
Glycerol	5263.0	19.81	5243.2

Design Data:

Total length	17.5 ft
Diameter	6 ft
Material of construction	Carbon steel

Utilities: Natural Gas Refrigerant, 10°F: 4839.4 tons/hr

Purchase Cost	$51,139
Bare Module Cost	$212,740

Comments: Uses refrigerant associated with Table 17.1 in Seider (Seider et al., 2017, p. 500)

Glycerol-Methanol Flash Vessel

Identification: Item: Flash Vessel; Item No.: P1-B; No. Required: 1

Function: Purify the glycerol out of the reactor by removing excess methanol

Operation: Continuous

Materials Handled:

	Feed	Distillate	Bottoms
Temperature (°C)	0	163.8	163.8
Pressure (bar)	1.38	0.345	0.345
Component mass flow (kg/hr)			
C14:0-ME	0	0	0
C16:0-ME	0	0	0
C16:1-ME	0	0	0
C18:0-ME	0	0	0
C18:1-ME	0	0	0
C18:2-ME	0	0	0
EPA-ME	0	0	0
DHA-ME	0	0	0
Methanol	4319.2	4298.9	20.27
Glycerol	5243.2	717.0	4526.2

Design Data:

Total height	12 ft
Diameter	3.5 ft
Material of construction	Carbon steel

Utilities: High Pressure Steam: 11985.6 lb/hr

Purchase Cost	$24,659
Bare Module Cost	$102,583

Comments:

FAME-Methanol Flash Vessel

Identification:

Item	Flash Vessel
Item No.	P1-C
No. Required	1

Function: Purify the FAME stream from the transesterification reactor

Operation: Continuous

Materials Handled:

	Feed	Distillate	Bottoms
Temperature (°C)	0	235.4	235.4
Pressure (bar)	1.38	1	1
Component mass flow (kg/hr)			
C14:0-ME	4178.3	128.9	4049.4
C16:0-ME	20461.3	305.4	20155.9
C16:1-ME	10909.9	153.5	10756.5
C18:0-ME	1493.1	10.67	1482.4
C18:1-ME	10295.1	71.73	10223.3
C18:2-ME	5436.8	38.08	5398.7
EPA-ME	13415.2	27.54	13387.7
DHA-ME	912.4	.823	911.6
Methanol	1174.11	1005.2	169.0
Glycerol	19.81	3.78	16.03

Design Data:

Total height	18 ft
Diameter	6 ft
Material of construction	Carbon steel

Utilities: High Pressure Steam: 47736.7 lb/hr

Purchase Cost	$51,895
Bare Module Cost	$215,883

Comments:

FAME-Hexene Flash Vessel

Identification:

Item	Flash Vessel
Item No.	P2-H
No. Required	1

Function: Separate the methyl Omega-3s from the 1-hexene stripping agent

Operation: Continuous

Materials Handled:

	Feed	Distillate	Bottoms
Temperature (°C)	35	106.9	106.9
Pressure (bar)	.965	.133	.133
Component mass flow (kg/hr)			
EPA-ME	4640.9	.3791	1348.1
DHA-ME	91.82	.0058	91.81
1-Hexene	3200.6	3183.7	16.92

Design Data:

Total height	12 ft
Diameter	3 ft
Material of construction	Carbon steel

Utilities: High Pressure Steam: 1089.35 lb/hr

Purchase Cost	$22,336
Bare Module Cost	$92,919

Comments and Drawings:

NaOH Stirred Tank Reactor

Identification: Item: Vertical Pressure Vessel; Item No.: P3-K; No. Required: 2

Function: Allow for reaction of FAME with NaOH to produce fatty acid carboxylates

Operation: Continuous

Materials Handled:

	Inlet	Inlet	Inlet	Outlet
Temperature (°C)	25	54.5	35.0	65
Pressure (bar)	1.21	1.21	1.50	1.01
Component mass flow (kg/hr)				
EPA-ME	1346.41	0.00	0.00	0.00
DHA-ME	91.57	0.00	0.00	0.00
Na-EPA Carboxylate	0.00	0.00	0.00	1380.25
Na-DHA Carboxylate	0.00	0.00	0.00	93.70
Water	0.00	812.14	2.46	814.59
Methanol	0.00	0.00	869.29	1014.18
1-Hexene	1.43	0.00	2.16	2.61
NaOH	0.00	217.02	0.00	36.17

Design Data:

Total height	4 ft
Diameter	13 ft
Material of construction	304-Stainless steel
Design pressure	2.43 barg

Utilities:

Total Purchase Cost	$113,101
Total Bare Module Cost	$470,498

Comments and Drawings: The vessel should be filled with nitrogen gas to maintain an inert atmosphere, and each vessel requires an agitator (turbine in a closed vessel, total purchase cost: $24,376, total bare module cost: $80,441). The mass balance does not close for 1-hexene due to limitations in modeling the process in Aspen, but the difference is negligible.

HCl Stirred Tank Reactor

Identification: Item: Vertical Pressure Vessel
Item No.: P3-P
No. Required: 2

Function: Allow for reaction of fatty acid carboxylates with HCl to produce Omega-3 fatty acids

Operation: Continuous

Materials Handled:

	Inlet	Inlet	Outlet
Temperature (°C)	127.5	25.0	25.0
Pressure (bar)	1.71	1.01	1.01
Component mass flow (kg/hr)			
Na-EPA Carboxylate	1380.25	0.00	0.00
Na-DHA Carboxylate	93.70	0.00	0.00
EPA	0.00	0.00	1286.73
DHA	0.00	0.00	87.82
Water	811.74	499.86	1485.85
Methanol	5.07	0.00	5.07
1-Hexene	0.11	0.00	0.11
NaOH	36.17	0.00	0.00
HCl	0.00	214.23	16.39
NaCl	0.00	0.00	317.11

Design Data:

Total height	3 ft
Diameter	10 ft
Material of construction	304-Stainless steel
Design pressure	2.43 barg

Utilities:

Total Purchase Cost	$82,595
Total Bare Module Cost	$343,595

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere, and each vessel requires an agitator (turbine in a closed vessel, total purchase cost: $15,121, total bare module cost: $49,900)

Omega-3-Water Decanter

Identification: Item: Horizontal Pressure Vessel
Item No.: P3-Q
No. Required: 1

Function: separate aqueous and organic phases leaving reactors P3-P

Operation: Continuous

Materials Handled:

	Inlet	Liquid 1	Liquid 2
Temperature (°C)	25	25	25
Pressure (bar)	1.2	1.2	1.2
Component mass flow (kg/hr)			
EPA	1286.73	1286.73	0.00
DHA	87.82	87.82	0.00
Water	1485.85	0.00	1485.85
Methanol	5.07	0.00	5.07
1-Hexene	0.11	0.00	0.11
NaOH	0.00	0.00	0.00
HCl	16.39	0.00	16.39
NaCl	317.11	0.00	317.11

Design Data:

Total length	3 ft
Diameter	12 ft
Material of construction	304-Stainless steel
Design pressure	2.43 barg

Utilities:

Purchase Cost	$29,785
Bare Module Cost	$123,904

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere

16.2 Columns

FAME-Silver Liquid-Liquid Extraction

Identification:

Item	Tray Column
Item No.	P2-F
No. Required	1

Function: Separate methyl Omega-3s from other FAMEs by complexation to free silver ions in methanol

Operation: Continuous

Materials Handled:

	Feed	Solvent	Extract	Raffinate
Temperature (°C)	35	35	35	35
Pressure (bar)	1.1	1.1	1	1
Component mass flow (kg/hr)				
C14:0-ME	464.1	0	0	464.1
C16:0-ME	2309.9	0	0	2309.9
C16:1-ME	1232.7	0	0	1232.7
C18:0-ME	169.9	0	0	169.9
C18:1-ME	1171.6	0	0	1171.6
C18:2-ME	618.7	0	0	618.7
EPA-ME	1534.2	0	1518.6	15.34
DHA-ME	104.5	0	103.4	0
Methanol	19.36	4954.3	4954.3	19.36
Glycerol	1.84	0	0	1.84
Silver Nitrate	0	4250.5	4250.5	0

Design Data:

Material of construction	Carbon steel
Height	12.5 ft
Diameter	6 ft
Theoretical Stages	2.20
Estimated Efficiency	0.25
Residence Time	25 minutes
Number of Stages	9

Purchase Cost	$48,668
Bare Module Cost	$272,921

Comments and Drawings:

FAME-Hexene Liquid-Liquid Extraction

Identification:

Item	Tray Column
Item No.	P2-G
No. Required	1

Function: Uncomplex methyl Omega-3s from silver ions in methanol by stripping with 1-hexene

Operation: Continuous

Materials Handled:

	Feed	Solvent	Extract	Raffinate
Temperature (°C)	35	35	35	35
Pressure (bar)	1.1	1.1	1	1
Component mass flow (kg/hr)				
EPA-ME	1518.6	0	1348.5	170.1
DHA-ME	103.4	0	91.82	11.6
Methanol	4954.3	0	0	4954.3
Silver Nitrate	4250.5	0	0	4250.5
1-Hexene	0	3200.6	3200.6	0

Design Data:

Material of construction	Carbon steel
Height	10 ft
Diameter	4 ft
Theoretical Stages	4.87
Estimated Efficiency	0.25
Residence Time	10 minutes
Number of Stages	20

Purchase Cost	$33,523
Bare Module Cost	$213,994

Comments and Drawings:

Omega-3-Methanol Distillation Column

Identification:

Item	Distillation Column
Item No.	P3-L
No. Required	1

Function: Separate methanol from feed which can be recycled to other processes

Operation: Continuous

Materials Handled:

	Feed	Distillate	Bottoms
Temperature (°C)	65.1	74.9	125.9
Pressure (bar)	1.8	1.5	1.78
Component mass flow (kg/hr)			
Na-EPA Carboxylate	1380.25	0.00	1380.25
Na-DHA Carboxylate	93.70	0.00	93.70
Water	814.59	2.85	811.74
Methanol	1014.18	1009.11	5.07
1-Hexene	2.61	2.51	0.11
NaOH	36.17	0	36.17

Design Data:

Number of trays	19
Feed stage	11
Total height	52 ft
Material of construction	304-Stainless steel
Diameter	2.5 ft
Tray spacing	2 ft
Molar reflux ratio	0.852

Utilities: Cooling water: 43,505.74 kg/hr, Steam at 100 psi: 1,163.95 kg/hr

Purchase Cost	$93,810
Bare Module Cost	$390,249

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere

16.3 Heat Exchangers

FAME Cooler

Identification: Item: Shell and Tube Heat Exchanger (1 Shell, 1 Pass)
Item No. P2-E
No. Required 1

Function: Cool the FAME stream entering the Omega-3 separation process

Operation: Continuous

Materials Handled:

	Hot Inlet	Cold Inlet	Hot Outlet	Cold Outlet
Temperature (°C)	235.4	32.2	35	48.9
Pressure (bar)	1.2	1	1.2	1
Component mass flow (kg/hr)				
C14:0-ME	464.1	0	464.1	0
C16:0-ME	2309.9	0	2309.9	0
C16:1-ME	1232.7	0	1232.7	0
C18:0-ME	169.9	0	169.9	0
C18:1-ME	1171.6	0	1171.6	0
C18:2-ME	618.7	0	618.7	0
EPA-ME	1534.2	0	1534.2	0
DHA-ME	104.5	0	104.5	0
Methanol	19.36	0	19.36	0
Glycerol	1.84	0	1.84	0
Water	0	44000	0	44000

Design Data:

Material of construction	Carbon steel
Surface area	334.5 ft^2
Heat duty	981.36 kW

Utilities: Cooling water: 44,000 kg/hr

Purchase Cost $12,618
Bare Module Cost $39,999

Comments:

1-Hexene Condenser

Identification:

Item	Shell and Tube Heat Exchanger (1 Shell, 1 Pass)
Item No.	P2-I
No. Required	1

Function: Cool the 1-hexene exiting the flash vessel before it is recycled to P2-G

Operation: Continuous

Materials Handled:

	Hot Inlet	Cold Inlet	Hot Outlet	Cold Outlet
Temperature (°C)	106.9	32.2	35	35.8
Pressure [bar]	0.133	1	0.133	1
Component mass flow (kg/hr)				
EPA-ME	0.3791	0	0.3791	0
DHA-ME	0.0058	0	0.0058	0
1-Hexene	3183.7	0	3183.7	0
Water	0	23390	0	23390

Design Data:

Material of construction	Carbon steel
Surface Area	67.56 ft^2
Heat Duty	112.4 kW

Utilities: Cooling water: 23,390 kg/hr

Purchase Cost	$11,357
Bare Module Cost	$36,001

Comments:

NaOH Reactor Water Jacket

Identification: Item: Vertical Pressure Vessel
Item No.: P3-KJ
No. Required: 2

Function: Flow with cooling water to transfer heat from reactive vessels P3-K

Operation: Continuous

Materials Handled:

	Inlet	Outlet
Temperature (°C)	32.2	48.8
Pressure (bar)	1.013	1.013
Component mass flow (kg/hr)		
Water	1917.25	1917.25

Design Data:

Total height	4.5 ft
Diameter	13.5 ft
Material of construction	Carbon steel
Design pressure	2.43 barg
Heat duty	37.14 kW

Utilities: Cooling water: 1917.25 kg/hr

Total Purchase Cost	$69,500
Total Bare Module Cost	$280,120

Comments and Drawings: utility requirement calculations shown in Appendix

Omega-3-Methanol Distillation Condenser

Identification:

Item	Shell and Tube Heat Exchanger (1 Shell, 1 Pass)
Item No.	P3-LC
No. Required	1

Function: Condense the vapor leaving from the top of distillation tower P3-C to liquid at its bubble point

Operation: Continuous

Materials Handled:

	Hot Inlet	Cold Inlet	Hot Outlet	Cold Outlet
Temperature (°C)	74.9	32.2	74.9	48.8
Pressure (bar)	1.5	1.01	1.5	1.01
Component mass flow (kg/hr)				
Water	5.29	43505.74	5.29	43505.74
Methanol	1870.12	0	1870.12	0
1-Hexene	4.64	0	4.64	0

Design Data:

Material of construction	Carbon steel
Surface Area	160.58 ft^2
Heat Duty	561.74 kW

Utilities: Cooling water: 47,503.13 kg/hr

Purchase Cost	$11,293
Bare Module Cost	$35,798

Comments and Drawings:

Methanol Cooler

Identification: Item: Shell and Tube Heat Exchanger (1 Shell, 1 Pass)
Item No.: P3-N
No. Required: 1

Function: Cool the methanol being recycled before sending it to base reactors P3-K

Operation: Continuous

Materials Handled:

	Hot Inlet	Cold Inlet	Hot Outlet	Cold Outlet
Temperature (°C)	74.9	32.2	35	48.8
Pressure (bar)	1.5	1.01	1.5	1.01
Component mass flow (kg/hr)				
Water	2.46	1873.59	2.46	1873.59
Methanol	869.29	0	869.29	0
1-Hexene	2.16	0	2.16	0

Design Data:

Material of construction	Carbon steel
Surface Area	43.63 ft^2
Heat Duty	35.94 kW

Utilities: Cooling water: 1,873.59 kg/hr

Purchase Cost	$12,048
Bare Module Cost	$38,192

Comments and Drawings:

HCl Reactor Water Jacket

Identification: Item: Vertical Pressure Vessel
Item No.: P3-PJ
No. Required: 2

Function: flow with chilled water to transfer heat from reactive vessels P3-P

Operation: Continuous

Materials Handled:

	Inlet	Outlet
Temperature (°C)	7.2	32.2
Pressure (bar)	1.013	1.013
Component mass flow (kg/hr)		
Water	6080.2	6080.2

Design Data:

Total height	3.5
Diameter	10.5
Material of construction	Carbon steel
Design pressure	2.43 barg
Heat duty	176.66 kW

Utilities: Chilled water: 6080.2 kg/hr

Purchase Cost	$23,712
Bare Module Cost	$98,642

Comments and Drawings: utility requirement calculations shown in Appendix

16.4 Pumps

FAMEs Pump to Splitter P2-D

Identification: Item: Centrifugal Pump; Item No.: P1-CP; No. Required: 1

Function: Pump the FAMEs from flash vessel P1-C to the splitter P2-D to separate streams for either biodiesel production or Omega-3 production

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	235.4	235.4
Pressure (bar)	1	1.2
Component mass flow (kg/hr)		
C14:0-ME	4049.4	4049.4
C16:0-ME	20155.9	20155.9
C16:1-ME	10756.5	10756.5
C18:0-ME	1482.4	1482.4
C18:1-ME	10223.3	10223.3
C18:2-ME	5398.7	5398.7
EPA-ME	13387.7	13387.7
DHA-ME	911.6	911.6
Methanol	169.0	169.0
Glycerol	16.03	16.03

Design Data:

Net work	0.711 kW
Material of construction	Carbon steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	8.9 ft

Utilities: Electricity: 0.711 kW

Purchase Cost	$4,611
Bare Module Cost	$15,215

Comments and Drawings:

FAME-Silver Pump

Identification:

Item	Centrifugal Pump
Item No.	P2-FP
No. Required	1

Function: Pump FAME-Silver extract stream coming from P2-F to P2-G

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	35	35
Pressure (bar)	1	1.1
Component mass flow (kg/hr)		
EPA-ME	1518.6	1518.6
DHA-ME	103.4	103.4
Methanol	4954.3	4954.3
Silver Nitrate	4250.5	4250.5

Design Data:

Net work	0.069 kW
Material of construction	Carbon steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	50 ft

Utilities: Electricity: 0.069 kW

Purchase Cost	$4,695
Bare Module Cost	$15,493

Comments and Drawings:

Silver Nitrate Recycle Pump

Identification:

Item	Centrifugal Pump
Item No.	P2-GP
No. Required	1

Function: Pump the silver nitrate methanol mixture from P2-G in a recycle loop back to the first column

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	35	35
Pressure (bar)	1	1.1
Component mass flow (kg/hr)		
EPA-ME	170.1	170.1
DHA-ME	11.6	11.6
Methanol	4954.3	4954.3
Silver Nitrate	4250.5	4250.5

Design Data:

Net work	0.063 kW
Material of construction	Carbon steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	50 ft

Utilities: Electricity: 0.063 kW

Purchase Cost	$5,808
Bare Module Cost	$19,167

Comments and Drawings:

Methyl Omega-3 Stream Pump

Identification:

Item	Centrifugal Pump
Item No.	P2-HP
No. Required	1

Function: Pump the separated Omega-3s to the P3-K

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	106.9	106.9
Pressure (bar)	0.133	1.2
Component mass flow (kg/hr)		
EPA-ME	1348.1	1348.1
DHA-ME	91.81	91.81
1-Hexene	16.92	16.92

Design Data:

Net work	0.169 kW
Material of construction	Carbon steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	30.05 ft

Utilities: Electricity: 0.169 kW

Purchase Cost	$8,448
Bare Module Cost	$27,878

Comments and Drawings:

1-Hexene Recycle Pump

Identification: Item: Centrifugal Pump; Item No.: P2-IP; No. Required: 1

Function: Pump the 1-hexene stream from the P2-I in a recycle loop back to P2-G

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	35	35
Pressure (bar)	1	1.1
Component mass flow (kg/hr)		
EPA-ME	0.3791	0.3791
DHA-ME	0.0058	0.0058
1-Hexene	3183.7	3183.7

Design Data:

Net work	0.0304 kW
Material of construction	Carbon Steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	50 ft

Utilities: Electricity: 0.0304 kW

Purchase Cost	$5,808
Bare Module Cost	$19,167

Comments and Drawings:

NaOH Tank Pump

Identification:

Item	Centrifugal Pump
Item No.	P3-JP
No. Required	1

Function: Pump aqueous NaOH mixture made in storage tank P3-J to base reactors P3-K

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	25	25
Pressure (bar)	1.01	1.21
Component mass flow (kg/hr)		
Water	812.14	812.14
NaOH	217.02	217.02

Design Data:

Net work	0.0159 kW
Material of construction	304-Stainless steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	5.51 ft

Utilities: Electricity: 0.0159 kW

Purchase Cost	$47,368
Bare Module Cost	$156,314

Comments and Drawings:

NaOH Reactor P3-K to Distillation Column P3-L Pump

Identification:

Item	Centrifugal Pump
Item No.	P3-KP
No. Required	1

Function: Pump contents from base reactors P3-K to distillation tower P3-L

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	65	65.1
Pressure (bar)	1.01	1.8
Component mass flow (kg/hr)		
Na-EPA Carboxylate	1380.25	1380.25
Na-DHA Carboxylate	93.70	93.70
Water	814.59	814.59
Methanol	1014.18	1014.18
1-Hexene	2.61	2.61
NaOH	36.17	36.17

Design Data:

Net work	0.301 kW
Material of construction	304-Stainless steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	32.09 ft

Utilities: Electricity: 0.301 kW

Purchase Cost	$12,505
Bare Module Cost	$41,267

Comments and Drawings:

Omega-3-Methanol Distillation Column Reflux Pump

Identification:

Item	Centrifugal Pump
Item No.	P3-LP
No. Required	1

Function: Pump contents from reflux accumulator P3-LD back into the top of distillation tower P3-L

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	74.9	74.9
Pressure (bar)	1.01	1.5
Component mass flow (kg/hr)		
Water	5.29	5.29
Methanol	1870.16	1870.16
1-Hexene	4.64	4.64

Design Data:

Net work	0.2231 kW
Material of construction	Carbon Steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	100 ft

Utilities: Electricity: 0.2231 kW

Purchase Cost	$6,017
Bare Module Cost	$19,857

Comments and Drawings:

HCl Tank Pump

Identification: Item: Centrifugal Pump
Item No.: P3-OP
No. Required: 1

Function: Pump aqueous hydrochloric acid solution made in P3-O to acid reactors P3-P

Operation: Continuous

Materials Handled:

	Feed	Outlet
Temperature (°C)	25	25
Pressure (bar)	1.01	1.41
Component mass flow (kg/hr)		
Water	657.81	657.81
HCl	214.23	214.23

Design Data:

Net work	0.043 kW
Material of construction	304-Stainless steel
Shaft rpm	3,600
Type	Centrifugal pump
Orientation	VSC
Head	17.61 ft

Utilities: Electricity: 0.043 kW

Purchase Cost	$33,157
Bare Module Cost	$109,417

Comments and Drawings:

16.5 Storage Tanks

NaOH Storage Tank

Identification:

Item	Storage Tank
Item No.	P3-J
No. Required	1

Function: Prepare an aqueous solution of sodium hydroxide to be used to carry out the base-promoted reaction in stirred tanks P3-K

Operation: Continuous

Materials Handled:

	Inlet	Inlet	Outlet
Temperature (°C)	25	25	54.5
Pressure (bar)	1.01	1.01	1.01
Component mass flow (kg/hr)			
Water	217.02	595.11	812.14
NaOH	217.02	0	217.02

Design Data:

Type	Cone roof
Volume	8,053 gal
Material of construction	304-Stainless steel
Holdup time	1 day

Utilities:

Purchase Cost	$56,572
Bare Module Cost	$226,287

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere

HCl Storage Tank

Identification:

Item	Storage Tank
Item No.	P3-O
No. Required	1

Function: Prepare an aqueous solution of hydrochloric acid to be used to carry out the acid-promoted reaction in stirred tanks P3-P

Operation: Continuous

Materials Handled:

	Inlet	Inlet	Outlet
Temperature (°C)	25	25	36.8
Pressure (bar)	1.01	1.01	1.01
Component mass flow (kg/hr)			
Water	499.86	157.95	657.81
HCl	214.23	0	214.23

Design Data:

Type	Cone roof
Volume	7,436 gal
Material of construction	304-Stainless steel
Holdup time	1 day

Utilities:

Purchase Cost	$54,305
Bare Module Cost	$217,222

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere

Omega-3 Storage Tank

Identification:

Item	Storage Tank
Item No.	P3-R
No. Required	1

Function: Store the Omega-3s being produced

Operation: Continuous

Materials Handled:

	To Tank
Temperature (°C)	25
Pressure (bar)	1.01
Component mass flow (kg/hr)	
EPA	1286.73
DHA	87.82

Design Data:

Type	Cone roof
Volume	111,157 gal
Material of construction	304-Stainless steel
Holdup time	7 days

Utilities:

Purchase Cost	$217,475
Bare Module Cost	$869,899

Comments and Drawings: vessel should be filled with nitrogen gas to maintain an inert atmosphere

Water Neutralization/Storage Tank

Identification:

Item	Storage Tank
Item No.	P3-S
No. Required	1

Function: Neutralize the acidity of and store the aqueous waste being produced

Operation: Continuous

Materials Handled:

	To Tank	To Tank	In Tank
Temperature (°C)	25	25	29.6
Pressure (bar)	1.01	1.01	1.01
Component mass flow (kg/hr)			
Water	1485.85	17.98	1511.93
Methanol	5.07	0	5.07
1-Hexene	0.11	0	0.11
NaOH	0	17.98	0
HCl	16.39	0	0
NaCl	317.11	0	343.38

Design Data:

Type	Cone roof
Volume	109,456 gal
Material of construction	304-Stainless steel
Holdup time	7 days

Utilities:

Purchase Cost	$215,762
Bare Module Cost	$863,048

Comments and Drawings:

17. Equipment Cost Summary

The cost of the equipment was calculated by using Equipment Costing spreadsheet provided by the Penn faculty, with spreadsheet inputs coming either from hand-calculations or calculated by the Aspen Process Economic Analyzer (Appendix). The purchase cost represents the expenses of purchasing the equipment. The bare module cost includes this purchase cost and also accounts for the expenses for installation materials and labor, freight, insurances, taxes, construction overhead, and contractor engineering. The bare module cost is estimated by multiplying the purchase cost by the bare module factor, and these factors were obtained by referencing Seider (Seider et al., 2017, p. 441). The prices calculated used a cost index of CE = 600, which was the default value used in the pricing spreadsheet provided by faculty advisors to price equipment. A different CE could have been chosen to reflect the present time, but a projected time for acting on this project was not provided to the project team since some out-of-scope portions of the project needed to be tested on a pilot scale.

The equipment used in this design and their calculated costs is listed in Table 17.1 and Table 17.2. Table 17.1 lists the cost of fabricated equipment, e.g., heat exchangers, separation columns, reaction vessels. Table 17.2 lists the costs of process machinery, i.e., pumps, and storage vessels. In general, the most expensive equipment is the equipment that falls within the Hydrolysis of Fames to Free Fatty Acids (Section 12.3, “P3”). This result is not only because of the quantity of equipment that is utilized for this portion of the process, but also because of the more expensive stainless steel used to build most of the equipment. All of the P1 and P2 equipment is made of the cheaper carbon steel, while a majority of the P3 equipment requires stainless steel to provide corrosion resistance against the strong base (NaOH) and strong acid (HCl) being used to conduct the requisite chemistry to produce Omega-3s.

The equipment size also plays a huge role in what the bare module costs of the equipment are. The most expensive equipment are storage tanks P3-R for Omega-3s and P3-S for wastewater. The most expensive fabricated equipment is reactor P3-K, which conducts the reaction of carboxylate with NaOH. All three pieces of equipment have large volumes to accommodate the large number of flows which either pass through or get stored. This demands more material for the construction of the equipment, which ultimately results in larger calculated costs.

One item to note is that spare parts were not considered, although they might be necessary. All the equipment which would be exposed to the significant amounts of corrosive material, i.e., HCl and NaOH, has been designed to be built with stainless steel. However, there is no guarantee that all these pieces will last the projected 20 years that this plant has been priced to operate. Additionally, some of the earlier processes deal with either very low pressures or very high temperatures which may pose some additional strain on the equipment. Thus, the profitability analysis to follow in later sections should consider that the equipment for this process was costed for an optimistic situation.

Table 17.1. Purchase Costs and Bare Module Costs for Fabricated Equipment

Unit ID	Unit Type	Equipment Description	Purchase Cost ($)	Bare Module Factor	Bare Module Cost ($)
P1-A	Decanter	FAME-Glycerol-Methanol Decanter	51,139	4.16	212,740
P1-B	Flash Vessel	Glycerol-Methanol Flash Vessel	24,659	4.16	102,581
P1-C	Flash Vessel	FAME-Methanol Flash Vessel	51,895	4.16	215,883
P2-E	Heat Exchanger	FAME Cooler	12,618	3.17	39,999
P2-F	Liquid-Liquid Extraction Column	FAME-Silver LLE	48,668	4.16	202,459
P2-G	Liquid-Liquid Extraction Column	FAME-Hexene LLE	33,523	4.16	139,456
P2-H	Flash Vessel	FAME-Hexene Flash Vessel	22,336	4.16	92,919
P2-I	Heat Exchanger	Hexene Condenser	11,357	3.30	36,001
P3-K	Reactor	NaOH Reactor	137,477	4.16	550,939
P3-KJ	Heat Exchanger	NaOH Reactor Water Jacket	69,500	4.16	289,120
P3-L	Distillation Column	Methanol Distillation Column	93,810	4.16	390,249
P3-LC	Heat Exchanger	Distillation Column P3-L Condenser	11,293	3.17	35,798
P3-LR	Heat Exchanger	Distillation Column P3-L Reboiler	53,090	3.17	168,297
P3-N	Heat Exchanger	Methanol Cooler	12,048	3.17	38,192
P3-P	Reactor	HCl Reactor	97,716	4.16	393,495
P3-PJ	Heat Exchanger	HCl Reactor Water Jacket	47,424	4.16	197,285
P3-Q	Decanter	Omega-3-Water Decanter	29,785	4.16	123,904

Table 17.2 Purchase Costs and Bare Module Costs of Storage Equipment and Process Machinery

Unit ID	Unit Type	Equipment Description	Purchase Cost ($)	Bare Module Factor	Bare Module Cost ($)
P1-CP	Pump	FAMEs Pump to Splitter P2-D	4,611	3.30	15,215
P2-FP	Pump	FAME-Silver Pump	4,695	3.30	15,493
P2-GP	Pump	Silver Nitrate Recycle Pump	5,808	3.30	19,167
P2-HP	Pump	P2-H to P3-K Pump	8,448	3.30	27,878
P2-IP	Pump	1-Hexene Recycle Pump	5,808	3.30	19,167
P3-J	Storage Tank	NaOH Tank	56,572	4.00	226,287
P3-JP	Pump	NaOH Tank Pump	47,368	3.30	156,314
P3-KP	Pump	P3-K to P3-L Pump	12,505	3.30	41,267
P3-LD	Storage Tank	Distillation Column P3-L Reflux Accumulator	15,783	4.16	65,659
P3-LP	Pump	Distillation Column P3-L Reflux Pump	6,017	3.30	19,857
P3-O	Storage Tank	HCl Tank	54,305	4.00	217,222
P3-OP	Pump	HCl Tank Pump	33,157	3.30	109,417
P3-R	Storage Tank	Omega-3 Storage	217,475	4.00	869,899
P3-S	Storage Tank	Water Neutralization/Storage	215,762	4.00	863,048

18. Fixed-Capital Investment Summary

The fixed capital investment for the plant was calculated using the procedure set out in Seider et al., 2017. All the costs included in the fixed capital investment are broken down in Table 18.1 below.

Table 18.1 Costs that Comprise Total Capital Investment (Seider et al., 2017)

Total bare-module costs for fabricated equipment	C_{FE}				
Total bare-module costs for process machinery	C_{PM}				
Total bare-module costs for spares	C_{spare}				
Total bare-module costs for storage and surge tanks	$C_{storage}$				
Total cost for initial catalyst charges	$C_{catalyst}$				
Total bare-module costs for computers and software, including distributed control systems, instruments, and alarms	C_{comp}				
Total bare-module investment, TBM		C_{TBM}			
Cost of site preparation		C_{site}			
Cost of service facilities		C_{serv}			
Allocated costs for utility plants and related facilities		C_{alloc}			
Total of direct permanent investment, DPI			C_{DPI}		
Cost of contingencies and contractor's fee			C_{cont}		
Total depreciable capital, TDC				C_{TDC}	
Cost of land				C_{land}	
Cost of royalties				C_{royal}	
Cost of plant startup				$C_{startup}$	
Total permanent investment, TPI					C_{TPI}
Working capital					C_{wc}
Total capital investment, TCI					C_{TCI}

In addition to the equipment and materials cost of the plant, costs relating to facilities, contractors, and land must be considered. These numbers make up a percentage of the total capital investment. The percent of each factor considered for the economics for the proposed plant are shown below in Table 18.2.

Table 18.2 Additional Costing Factors for Total Capital Investment (Seider et al., 2017)

Cost of Site Preparations:	5.00%	of Total Bare Module Costs
Cost of Service Facilities:	5.00%	of Total Bare Module Costs
Cost of Contingencies and Contractor Fees:	18.00%	of Direct Permanent Investment
Cost of Land:	2.00%	of Total Depreciable Capital
Cost of Plant Start-Up:	10.00%	of Total Depreciable Capital

The numbers in Table 18.1 and Table 18.2 applicable for our plant were tabulated using the profitability spreadsheet made by Brian K. Downey using the costing procedures outlined in Seider et al., 2017. The breakdown of all of the costs necessary for the development and running of the plant are listed below in Table 18.3.

Table 18.3 Total Permanent Investment Breakdown for Proposed Plant

Investment Summary

Total Bare Module Costs:				
Fabricated Equipment	$	-		
Process Machinery	$	3,031,145		
Spares	$	-		
Storage	$	2,176,456		
Other Equipment	$	-		
Catalysts	$	2,005,827		
Computers, Software, Etc.	$	-		
Total Bare Module Costs:			**$**	**7,213,428**
Direct Permanent Investment				
Cost of Site Preparations:	$	360,671		
Cost of Service Facilities:	$	360,671		
Allocated Costs for utility plants and related facilities:	$	-		
Direct Permanent Investment			**$**	**7,934,771**
Total Depreciable Capital				
Cost of Contingencies & Contractor Fees	$	1,428,259		
Total Depreciable Capital			**$**	**9,363,030**
Total Permanent Investment				
Cost of Land:	$	187,261		
Cost of Royalties:	$	-		
Cost of Plant Start-Up:	$	936,303		
Total Permanent Investment - Unadjusted			$	10,486,594
Site Factor				1.00
Total Permanent Investment			**$**	**10,486,594**

As seen in Table 18.3, there is a large amount of money set aside for the purchase of catalysts. Although labeled catalysts for profitability, the price of the catalysts derives from the chemicals used throughout the process that are then recycled once the process is up and running. Since these chemicals do not require constant replenishment, for profitability, they are listed under catalysts and are a one-time cost. The specific chemicals being purchased and their total overall costs are listed in Table 18.4. The costs of each chemical can be found in the database section as Table 11.4.

Table 18.4 Summary of Capital Chemical Costs

Type of Overhead	Cost
Required Chemicals	**$2,006,439.82**
Silver Nitrate	$1,700,180.59
1-Hexene	$4,640.93
Methanol	$2,516.10
Nitrogen	$299,102.20
Equipment	**$2,173,210.66**
Total Additional Capital Investment	**$4,179,650.48**

In order to determine the total capital investment for the plant, the permanent investment and working capital must be considered. The working capital accounts for thirty days of accounts receivable, cash reserves, and accounts payable, with 4 days of biodiesel inventory and 2 days of raw materials inventory. The total capital investment calculations are shown below in Table 18.5. It is expected that the total capital investment for the plant will be $12.1 MM.

Table 18.5 Total Capital Investment Calculation for Proposed Plant

Working Capital

	2021	2022	2023
Accounts Receivable	$ 14,889,069	$ 7,444,535	$ 7,444,535
Cash Reserves	$ 350,375	$ 175,187	$ 175,187
Accounts Payable	$ (17,356,693)	$ (8,678,346)	$ (8,678,346)
Biodiesel Inventory	$ 1,985,209	$ 992,605	$ 992,605
Raw Materials	$ 1,144,835	$ 572,417	$ 572,417
Total	**$ 1,012,796**	**$ 506,398**	**$ 506,398**
Present Value at 15%	*$ 880,692*	*$ 382,910*	*$ 332,965*

Total Capital Investment **$ 12,083,160**

19. Operating Cost—Cost of Manufacture

The operating cost of the plant is comprised of several subcategories. This plant is very large and will produce 547,830 US-tons of biodiesel, 12,000 US-tons of Omega-3 fatty acids, and 39,683 US-tons of crude glycerol per year. This production level satisfies 10% of the current biodiesel market, 30% of the United States Omega-3 market in 2024, and 6% of the current glycerol market. Because of the large throughput of the plant, a large category of operating cost is the raw materials required. Although many of the chemicals will be purchased once and then recycled, other chemicals are used up in the reaction and must be continuously purchased as raw materials in the process. Because the proposed plant is only a portion of a larger process, the raw material prices for the FAMEs oil coming out of the reactor could not be easily estimated. Therefore, for profitability calculations, the FAMEs purchase price was varied to observe the response in the economics of the plant. This calculation is discussed further in Section 21. However, for the example case presented in the tables below, the FAMEs had an estimated purchase cost of $0.75/kg. The raw materials required for the plant are summarized in Table 19.1.

Table 19.1 Summary of Raw Material Costs for Proposed Plant

Feedstock Costs	Cost per Year (USD)
FAMEs Oil from Reactor	$77,858.30
1-Hexene	$189,806.55
NaOH	$1,111,668.25
HCl	$562,978.67
Total Feedstock	$1,942,311.77

In addition to raw materials, the utilities for the plant are a large factor in the operating cost. High-pressure steam will perform most of the heating for the process, and refrigerant will be purchased for the cooling of the decanter. The heat exchangers require large amounts of cooling water, and the reactors require process water. The block by block breakdown of utility requirements can be found in Section 14. The utilities used and their total costs are summarized below in Table 19.2.

Table 19.2 Summary of Utility Costs for Proposed Plant

Utility	Cost per Year (USD)
Electricity	$872.80
Refrigeration	$895,726.47
High Pressure Steam	$4,014,407.31
Cooling Water	$14,510.22
Process Water	$1,254.73
Chilled Water	$24,572.43
Total Utility Costs	$4,951,343.96

In addition to the costs attributed to the purchase of raw materials and utilities, the general expenses of the plant must also be considered to determine the total variable costs of the plant. These expenses are tied to product sales and are sensitive to fluctuations in the market. Therefore, they are considered variable costs and are factored into the operating costs of the plant. Table 19.3 summarizes the total variable costs for this proposed plant for a FAME purchase price of $0.75/kg.

Table 19.3 Variable Costs of Plant

Variable Cost Summary			
Variable Costs at 100% Capacity:			
General Expenses			
Selling / Transfer Expenses:		$	12,076,690
Direct Research:		$	19,322,703
Allocated Research:		$	2,012,782
Administrative Expense:		$	8,051,126
Management Incentive Compensation:		$	5,031,954
Total General Expenses		$	46,495,255
Raw Materials	$0.934225 per kg of Biodiesel		$464,294,192
Byproducts	$0.244511 per kg of Biodiesel		($121,518,019)
Utilities	$0.010019 per kg of Biodiesel		$4,979,354
Total Variable Costs		**$**	**394,250,782**

In addition to the variable costs of the plant, there are several fixed costs that pertain specifically to operating the plant. These costs are attributed to labor, maintenance, and other general expenses. The fixed operating costs, summarized in Table 19.4 below, were calculated using the methods explained in Seider et al., 2017, and the profitability spreadsheet prepared by Brian K. Downey and provided by the Penn faculty who assisted us with this project.

Table 19.4 Summary of Fixed Operating Cost for Proposed Plants

Fixed Cost Summary		
Operations		
Direct Wages and Benefits	$	1,081,600
Direct Salaries and Benefits	$	162,240
Operating Supplies and Services	$	64,896
Technical Assistance to Manufacturing	$	780,000
Control Laboratory	$	845,000
Total Operations	**$**	**2,933,736**
Maintenance		
Wages and Benefits	$	421,336
Salaries and Benefits	$	105,334
Materials and Services	$	421,336
Maintenance Overhead	$	21,067
Total Maintenance	**$**	**969,074**
Operating Overhead		
General Plant Overhead:	$	125,706
Mechanical Department Services:	$	42,492
Employee Relations Department:	$	104,460
Business Services:	$	131,018
Total Operating Overhead	**$**	**403,676**
Property Taxes and Insurance		
Property Taxes and Insurance:	$	187,261
Other Annual Expenses		
Rental Fees (Office and Laboratory Space):	$	-
Licensing Fees:	$	-
Miscellaneous:	$	-
Total Other Annual Expenses	**$**	**-**
Total Fixed Costs	**$**	**4,493,747**

20. Other Important Considerations

This process was designed with attention to choosing safe materials whenever possible. Safety had a role when deciding to use 1-hexene in the FAME separation portion of the process. Other alternatives, such as diethyl ether, were either more flammable at extraction conditions or less effective than 1-hexene (Section 25.3). Unfortunately, the selection of safe reactants could not always be chosen, and the process does require the use of NaOH, a strong base, and HCl, a strong acid. Each has their safety hazards but are required for the chemistry this process demands (Section 25.3). These reactants are often used at relatively low temperatures, not exceeding 130°C for most of the process and are used with equipment with a large enough corrosion thickness to account for their use to minimize the dangers they pose (Seider et al., 2017, p. 466).

The location of the plant, while out of scope, is also another consideration when determining the costs of this process. The cultivation of algae requires a large amount of land, which can be used to form the necessary algal cultivators, a large amount of salt water, and enough sunlight to grow well. The profitability analysis of this design is based on the economic regulations of the United States. If the designed plant were to be built within the United States, the Gulf Coast would be a good location to consider and was the location factor used in all profitability. This region of the US receives adequate amount sunlight, has a proper temperature range for algal lipid production, and is close enough to provide a source of salt water to an algal raceway (Moody et al., 2014). Alternative locations would have to meet these criteria and would ideally be cheaper than trying to build a large plant within the United States.

21. Profitability Analysis—Business Case

The purpose of this project was to sell byproducts in order to reduce the overall cost of producing biodiesel using the suggested process. Our proposed plant can produce 547,830 US-tons of biodiesel, 12,000 US-tons of Omega-3 fatty acids, and 39,683 US-tons of crude glycerol per year. This production level satisfies 10% of the current biodiesel market, 30% of the United States Omega-3 market in 2024, and 6% of the current glycerol market. Because the proposed plant is part of a larger process, it is important that the profitability of the plant be considered from multiple angles. The economics of the plant depends mainly on three different variables: the purchase price of the FAMEs stream coming out of the transesterification reactor, the sales price of the Omega-3s, and the sales price of the biodiesel. Normally the price of the feedstocks of a process would generally be known. However, because the feedstock for this process (FAMEs exiting the transesterification reactor) is a product of another portion of the process it was difficult to determine a set price with the data currently available. Therefore, several different scenarios were analyzed in order to determine how the plant could be profitable.

Each different costing scenario was input into a profitability analysis spreadsheet which determined the profitability of the plant at the input costing conditions. Each scenario was defined as a profitability analysis that varied the prices of the three variables defined above. The scenarios did not affect the capital expenditures, the change in prices only varied the operating costs of the plant. A scenario selling biodiesel for $2.80 per gallon and purchasing FAMEs at $0.75 per kilogram will be used as an example to demonstrate the spreadsheet's calculations. In order to first determine the capital expenditures of the plant, the equipment costs, discussed in Section 17, were inputted into the worksheet. In addition to equipment, any chemicals required in large amounts that would then be recycled during the process had to be costed as capital investments and were inputted as catalysts. The resulting spreadsheet, shown in Appendix 25.2.2 lists all the equipment required and determines the total equipment bare module cost for the plant. The variable costs and total investments discussed in Section 19 were also input into the spreadsheet. Then, the parameters of the plant were defined. The first half of general input, shown in Figure 21.1 below, defined the location, operating days, and production rate of the plant. The lifetime of the plant, as well as the time for design and construction, were chosen as well as the tax rate (24%) and depreciation value (5 year MACRS) used to determine

profitability. For the proposed plant, the design and construction were both one year, and the lifetime of the plant was set at 20 years.

General Information

Process Title:	**Algae to Biofuel**
Product:	**Biodiesel**
Plant Site Location:	**Gulf Coast**
Site Factor:	**1.00**
Operating Hours per Year:	**7919**
Operating Days Per Year:	**330**
Operating Factor:	**0.9040**

Product Information

This Process will Yield

62,758	kg of Biodiesel per hour
1,506,192	kg of Biodiesel per day
496,983,112	kg of Biodiesel per year

Price **$0.81 /kg**

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2020	Design		0.0%		
2021	Construction	100%	0.0%		
2022	Production	0%	45.0%	20.00%	$0.81
2023	Production	0%	67.5%	32.00%	$0.81
2024	Production	0%	90.0%	19.20%	$0.81
2025	Production		90.0%	11.52%	$0.81
2026	Production		90.0%	11.52%	$0.81
2027	Production		90.0%	5.76%	$0.81

Figure 21.1 General Input Specifications for Plant Operation

In addition to the plant specifics, the spreadsheet also considers the expenses incurred from raw materials, utilities, and the sale of byproducts. For this plant, biodiesel was defined as the product, and both glycerol and Omega-3s were defined as byproducts. The ratio of byproducts produced per kilogram of biodiesel is inputted into the spreadsheet as well as the sales price for each of the byproduct. The process is then repeated with raw materials and utilities, such that the required amounts per kilogram of biodiesel and the costs are inputted into the worksheet. These inputs are summarized in Table 21.1 below. Utilities and raw materials are both considered variable costs of the plant. Byproducts, although a portion of the sales revenue are considered as a discount on the variable costs of the system.

Table 21.1 Spreadsheet Input for Raw Materials, Byproducts, and Utilities

Raw Materials						
	Raw Material	**Unit**	**Required Ratio**		**Cost of Raw Material**	
1	1- Hexene	kg	0.00	kg per kg of Omega-3 Fatty Acids	$1.450	per kg
2	NaOH	kg	0.01	kg per kg of Omega-3 Fatty Acids	$0.300	per kg
3	HCL	kg	0.01	kg per kg of Omega-3 Fatty Acids	$0.100	per kg
4	FAMEs Oil	kg	1.24	kg per kg of Omega-3 Fatty Acids	$0.750	per kg
	Total Weighted Average:				$0.934	per kg of Omega-3 Fatty Acids
Byproducts						
	Byproduct	**Unit**	**Required Ratio**		**Byproduct Selling Price**	
1	Glycerol	kg	0.07244	kg per kg of Omega-3 Fatty Acids	$0.245	per kg
2	Omega-3s	kg	0.021911	kg per kg of Omega-3 Fatty Acids	$10.350	per kg
	Total Weighted Average:				$1.113	per kg of Omega-3 Fatty Acids
Utilities						
	Utility:	**Unit:**	**Required Ratio**		**Utility Cost**	
1	High-Pressure Steam	lb	1.0099	lb per kg of Omega-3 Fatty Acids	$8.000E-03	per lb
2	Low Pressure Steam	lb	0	lb per kg of Omega-3 Fatty Acids	$7.000E-03	per lb
3	Process Water	gal	0.00317	gal per kg of Omega-3 Fatty Acids	$8.000E-04	per gal
4	Cooling Water	gal	0.483	gal per kg of Omega-3 Fatty Acids	0.0001	per gal
5	Electricity	kWh	2.51958E-05	kWh per kg of Omega-3 Fatty Acids	$0.070	per kWh
6	Refrigerant	ton-day	0.000917	ton-day per kg of Omega-3 Fatty Acids	$2.000	per ton-day
7	Chilled Water	ton-day	3.32E-05	ton-day per kg of Omega-3 Fatty Acids	$1.500	per ton-day
8	Wastewater Treatment	lb organic	0.0001817	lb organic per kg of Omega-3 Fatty Acids	$0.150	per lb organic
	Total Weighted Average:				$0.010	per kg of Omega-3 Fatty Acids

Once all the cost requirements of the plant were input into the spreadsheet, the profitability of the plant could be determined by assessing its cash flow, return on investment

(ROI), the internal rate of return (IRR), and net present value (NPV). For the first condition run, the sale price of the biodiesel was set at $0.81 per kg ($2.80 per gallon), and the FAMEs purchase price was set at $0.75 per kg. The Omega-3 sales price was then varied until the plant had an IRR of 15.08%. The IRR is calculated iteratively; it is the theoretical rate of return of the project if the net present value was zero. For this scenario, the Omega-3 price was iteratively determined to be $10.35 per kilogram. At this set of prices, the cost summary, shown in full in Appendix 23.2.2, shows that the sale of the Omega-3s reduced the variable costs of the plant by $121.5 million and that the total capital investment for the proposed plant would be $12 million. The cash flow of the plant is shown on the next page as Figure 21.2.

Year	Percent Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Taxable Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 15%
2020	0%		-	-	-	-	-	-	-	-	-	-	-
2021	0%		-	(10,486,600)	(1,012,800)	-	-	-	-	-	-	(11,499,400)	(9,999,500)
2022	45%	$0.81	181,150,300	-	(506,400)	(177,412,900)	(4,493,700)	(1,872,600)	(2,628,900)	604,600	(2,024,200)	(658,000)	(10,497,000)
2023	68%	$0.81	271,725,500	-	(506,400)	(266,119,300)	(4,493,700)	(2,996,200)	(1,883,700)	433,200	(1,450,400)	1,039,300	(9,813,600)
2024	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	(1,797,700)	1,183,500	(272,200)	911,300	2,709,000	(8,264,700)
2025	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	(1,078,600)	1,902,600	(437,600)	1,465,000	2,543,600	(7,000,100)
2026	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	(1,078,600)	1,902,600	(437,600)	1,465,000	2,543,600	(5,900,400)
2027	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	(539,300)	2,441,900	(561,600)	1,880,300	2,419,600	(4,990,800)
2028	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(4,240,400)
2029	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(3,587,800)
2030	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(3,020,400)
2031	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(2,527,000)
2032	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(2,098,000)
2033	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(1,724,900)
2034	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(1,400,400)
2035	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(1,118,300)
2036	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(873,000)
2037	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(659,700)
2038	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(474,200)
2039	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(312,900)
2040	90%	$0.81	362,300,700	-	-	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	2,295,600	(172,600)
2041	90%	$0.81	362,300,700	-	2,025,600	(354,825,700)	(4,493,700)	-	2,981,200	(685,700)	2,295,600	4,321,100	56,900

Figure 21.2 Cash Flow Summary of Example Case for Plant

Because the sales price of Omega-3s was calculated for 15% IRR, you can see that the NPV is only $57,000. This NPV is the baseline of profitability for a plant with these parameters. If the sales price of either the biodiesel of Omega-3s were raised higher, the plant would become even more profitable. The case shown here estimates the bare minimum of profitability for a plant at these conditions.

The scenario just discussed, clearly shows that the plant could be profitable and reduce the sale price of the biodiesel significantly from $4.34 per gallon. Because of the variability in purchase and sales price, this is one of the possibly many scenarios for which the plant could be profitable. However, it is first important to consider the additional operating and capital investment that would be required to separate and convert the methyl EPA and DHA into their sellable form. The additional investment was determined by evaluating the equipment, utilities, and raw materials required to separate and purify the Omega-3s. The results, summarized in Table 21.2 and Table 21.3 below, demonstrate the costs of separating and refining the Omega-3s relative to the cost already required for refinement of the biodiesel. Table 21.2 shows the equipment and feedstock requirements that pertain only to the portion of the plant which is necessary for the byproduct purification. As a result, Table 21.2 shows the difference in the total capital investment required to separate the EPA and DHA. Although $4.2 million dollars is a large amount of capital, when you consider that one year of Omega-3 production will reduce the variable costs of the plant by anywhere from $172 to $553 million dollars, the additional capital investment seems well worth it as it will be paid back within the first year of plant operation.

Table 21.2 Capital Investment Costs for Omega-3 Separation and Purification Section

Type of Overhead	Cost
Required Chemicals	**$2,006,439.82**
Silver Nitrate	$1,700,180.59
1-Hexene	$4,640.93
Methanol	$2,516.10
Nitrogen	$299,102.20
Equipment	**$2,173,210.66**
Total Additional Capital Investment	**$4,179,650.48**

In addition to the more expensive capital investment, the separation and purification of the Omega-3s will also increase the variable costs for the plant every year. Because of the

additional feedstocks and utilities used, the Omega-3 process significantly increases the cost of utilities per year. The Omega-3 production requires an additional $4.7 million dollars in utilities per year, making the total utilities for the proposed plant cost $10.6 million dollars per year, as detailed in Table 21.3. It is important to note here that this table does not list all the utilities required to create the biodiesel, but only the utilities required to refine the products of the transesterification reactor. The utilities of the purification are shown here to demonstrate the relative magnitude of utilities required for the separation of the Omega-3s. Even though the magnitude of annual utility costs is quite high, the preliminary analysis for the plant presented in this design suggests that once again the increased costs annually are worth the increased sales.

Table 12.3 Annual Cost Comparison Between Biodiesel Plant Requirements and Costs Necessary Only for Omega-3 Production

	Yearly Cost for Process	
Utility	Required for Biodiesel Production	Required for Only Omega-3 Production
Electricity	$551.22	$321.58
Refrigeration	$895,726.47	$0.00
High Pressure Steam	$3,783,546.73	$230,860.58
Cooling Water	$0.00	$14,510.22
Process Water	$0.00	$1,254.73
Chilled Water	$0.00	$24,572.43
Total Utility Costs	**$4,679,824.42**	**$271,519.54**
Feedstock Costs		
FAMEs Oil from Reactor	$77,858.30	$0.00
1-Hexene	$0.00	$189,806.55
NaOH	$0.00	$1,111,668.25
HCl	$0.00	$562,978.67
Total Feedstock	**$77,858.30**	**$1,864,453.47**
Total Yearly Costs	**$4,757,682.72**	**$2,135,973.01**

After establishing how Omega-3 separation affected the capital investment, several scenarios were run to determine how varying the purchases and sales prices of the FAMEs, Omega-3s, and biodiesel in the plant would affect the profitability. It is important to note that the capital investments remained the same throughout all scenarios tested. This means neither the equipment costs or the throughput in the process were varied at all from the numbers explained previously. Varying the costs of the raw materials and sales prices changed the variable costs only. Like the example scenario explained earlier, two of the three variables were set for each scenario, and the price of the third was iterated until profitable economics came back. The first analysis varied the incoming FAMEs price to see how it would affect the economics of the plant. Because this project hopes to be competitive with the previously mention HTL process from the Department of Energy's PNNL, the goal number for FAMEs selling price has been $2.80 per gallon. This number, which translates to $0.81 per kilogram, was used as the set price for the first profitability analysis scenarios. The FAMEs purchase price was then varied at ten cent intervals. The Omega-3 sales price was then adjusted until the purchase price, and the

corresponding sale price resulted in an IRR of 15%. Because the price is limited in adjustment to two decimal places and the prices made such a large difference on the IRR, the uncertainty in IRR was set to 1%.

Figure 21.3 below illustrates the relationship between FAMEs purchase price and required Omega-3s sale price for a plant with an IRR of 15% that sells FAMEs at $2.80 per gallon. As you can see from the graph, as expected the relationship is linear. It is important to note that selling the Omega-3 byproducts means that the final biodiesel product can be sold for a lower price than it is purchased for per kg and still be profitable. This gives the proposed process significantly more leeway with how it produces its FAMEs oils and whether it purchases FAMEs from a separate location and ships them to the plant for Omega-3 separation. Because the Omega-3s are expected to sell for such a high cost, the plant could possibly absorb the additional cost of being off sight from the algae de-oiling process or possibly even purchasing products from other companies instead of producing their own algae and FAMEs. This is promising for the plant as it gives future designers more options when choosing locations as well as a buffer in variable costs. It also creates a goal price for developers of the algae growth and separation stages to hit such that the final products of their plants could sell for such a low price.

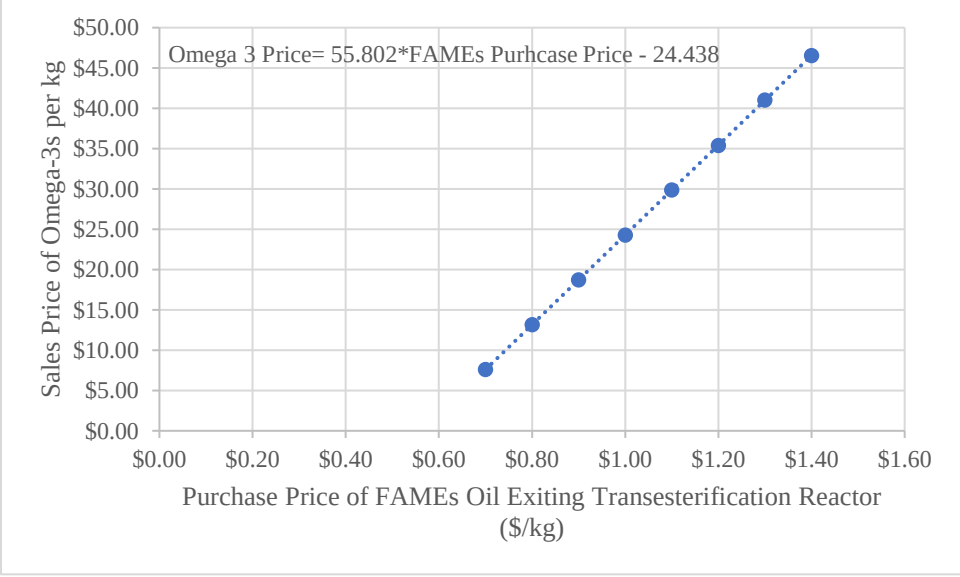


Figure 21.3 Effect of Varying FAMEs Purchase Price on Required Omega-3 Sales Price The graph below illustrates the necessary sales price of Omega-3s for varying purchase price of the FAMES mixture exiting the transesterification reactor for the plant to sell biodiesel at $2.80 per gallon. This number was chosen as it is the reported price that the PNNL HTL process can produce biodiesel at. The Omega-3 sales price chosen was the price at which the plant was profitable and had an IRR of approximately 15% which was found iteratively by keeping the sales and purchase price of FAMEs constant and varying the sales price until the plant was profitable.

Although the price of the transesterification reactor products is quite important to the feasibility of the plant, the main purpose of this project was to determine how separating the Omega-3s from the FAMEs could influence the price of the biodiesel. This was approached from two different directions. The first direction, already explored in Tables 21.2 and 21.3, determined how adding the equipment and resources necessary to separate and purify the Omega-3s for sale affected the total capital investments and annual costs of the plant. Although expensive, the costs were deemed worth it relative to the potential sales revenue.

The second method used to determine the Omega-3s effect on the plant's economics was by evaluating how much the byproduct sales could reduce costs per kilogram of biodiesel. This was determined by finding the sales revenue from the Omega-3s produced in an hour and dividing this number by the mass of biodiesel produced in an hour. Since the price of Omega-3s on the market could not be easily identified, a range of possible sales prices was estimated to be between $15 and $120 dollars. The total possible reduction in price was then calculated for the biodiesel at $5 price increments for the entire range of prices. The results, shown below in Figure 21.4 demonstrate how much the sale of Omega-3s can affect the price of the biodiesel. Even though only 1,375 kg/hr of Omega-3s will be sold compared to 62,758 kg/hr of biodiesel, the revenue from selling the Omega-3s can reduce the cost of the biodiesel by as much as $2.65 per kilogram which is more than double what the price per kilogram is for the biodiesel with no Omega-3 sales. Obviously, this number does not have real life applications outside of the model. Therefore, the next step was to determine the possible sales price of the biodiesel based on varied Omega-3 revenue.

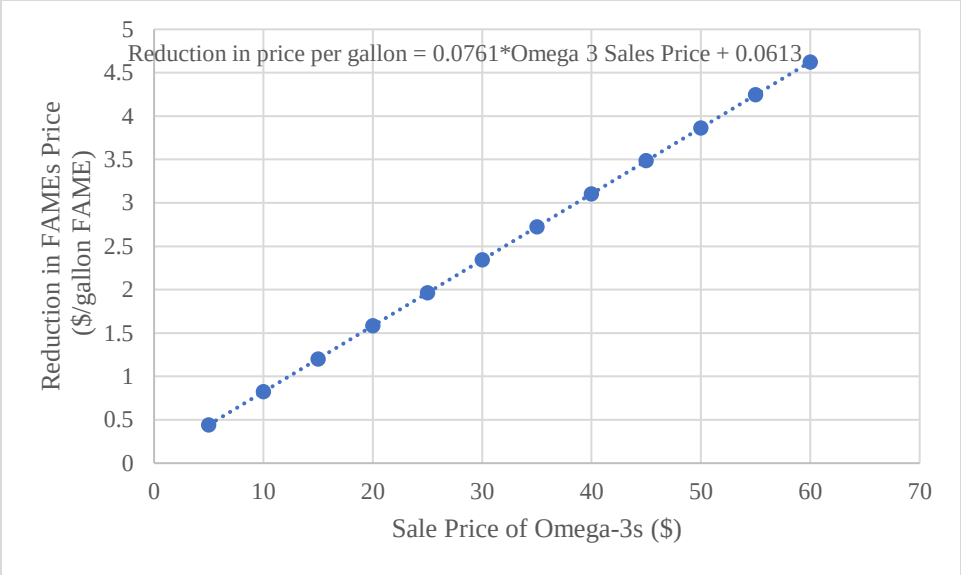


Figure 21.4 Effect of Omega-3s Sale Price on Possible Reduction in Biodiesel Price The maximum discount in biodiesel sales price per gallon was determined by finding the sales of the Omega-3s and normalizing the price by dividing by the amount of FAMEs produced in the same time frame. This was then graphed to show how much the fuel price could be reduced by Omega-3 sales. It is important to note that this value is independent of the FAMEs purchase price. However, it is only applicable if the price is kept constant when comparing biodiesel and Omega-3 sales prices.

Several economic scenarios were run to determine the potential sale price of the biodiesel at varying Omega-3 prices to provide the overall process with more information about potential pricing. For these scenarios, the FAMEs oil purchase cost was held constant at $0.75 per kilogram. This number was chosen somewhat arbitrarily based on the purchase price of FAMEs oil that would be profitable selling at $4.34 per gallon with no Omega-3s sales. Although this is not an exact number because of the increased number of utilities required for the Omega-3 separation, it allowed us to create an approximate estimate for sales prices based from the data available. The results of the various scenarios are listed in Table 21.4. The prices presented are the values based off a FAMEs purchase price of $0.75 per kilogram and a plant IRR of 15%. There is once again a linear relationship between the price of the Omega-3s and the potential sales price of the biodiesel. It is important to note that selling the Omega-3s at a price even as low as $20 per kilogram can reduce the price of the biodiesel to below $2 at this purchase price.

Table 21.4 Potential Profitable Sales Price of Biodiesel for Varying Omega-3 Sales

Biodiesel Sale Price per Gal	Omega-3 Sales Price per Kilogram
$0.35	$38.43
$0.69	$34.45
$1.04	$30.51
$1.39	$26.56
$1.74	$22.61
$2.08	$18.65
$2.43	$14.70
$2.78	$10.75
$3.12	$6.79
$3.47	$2.84

Although all of the profitability measures taken are very positive about the viability of reducing the biodiesel costs by selling Omega-3s, it is important to note the variables and oversights that must be taken into account when thoroughly analyzing the profitability of the entire proposed process that will include our plant design. When the plant is run, the cost of growing, harvesting, and flocculating the algae must be considered. In addition, many of the streams in our proposed plant are meant to be recycled to earlier portions of the process. When this is taken more thoroughly into account, it should significantly reduce the amount of feedstock required for the overall process. In addition, before the plant is built, buyers of the Omega-3s must be identified and the logistics and costs associated with shipping and transportation the material to these buyers must be considered to determine a more refined costing analysis for the process. However, initial profitability analysis for this project are very promising and indicate that the separation of Omega-3s is significantly less expensive than the cost at which they can be sold. This revenue may be able to reduce the sale price of biodiesel by an impressive amount.

22. Conclusions and Recommendations

The purpose of this design project was to propose a process design for the separation of the byproducts of the algae to biodiesel process to be sold to reduce the overall cost of the biodiesel produced. The proposed plant separates and purifies the glycerol and Omega-3 byproducts. This was achieved by creating a plant that would send 11.5% of the FAMEs it produced to a separation comprised of two liquid-liquid extraction columns. The methyl Omega-3s produced would then be converted into their carboxylic acid form through an acid-base reaction. Because of the number of economic variables in the plant, a variety of profitability scenarios were run to determine at which conditions the plant would be profitable, and when the plant would be able to produce biodiesel at lower costs. The profitability analysis is quite promising and suggests that if the FAMEs oil that enters from the transesterification reactor can be produced or purchased at a reasonable price, the Omega-3 sales can easily reduce the cost of the biodiesel produced by the plant. Although this design proposal is quite promising, it is important to note its limitations and the steps that would have to be taken before this plant becomes a reality.

The development of this proposed plant was limited significantly by the lack of research available about the separation of FAMEs, as well as data on FAMEs characteristics including solubility data, specific decomposition temperatures, and other important quantitative data. Although there was significant research available about separating FAMEs using silver complexation in chromatography, little research has gone into the separation of FAMEs at large scale. Therefore, it would be essential for the future plant that a study be run at a pilot scale of the proposed LLE process. Because no mass transfer data was available, it is highly likely that the actual stage size and stage requirements of the proposed LLEs may differ. The design proposed herein would benefit greatly from quantitative data demonstrating the viability of the research used at industrial scales.

The decision to model the hydrolysis of FAMEs to Omega-3 fatty acids was informed through a compilation of the work performed by various research groups. An ideal source to model this portion would have been an industrial scale reactor which hydrolysis fatty acid methyl esters to carboxylic acids. The closest sources to providing this information were based on the hydrolysis of triglycerides directly to fatty acids primarily in small, laboratory scales, although one source (Kywe & Mya, 2009) managed to conduct some experiments on an industrial scale

reactor. As a result, information such as the kinetics of the reactions was unknown, and the process had to be modeled by extrapolating residence times within reactors from reaction times. Additionally, since the starting material is the triglyceride rather than the methyl ester, it is possible that excess reagents are being used. While this use of excess reagent guarantees a high conversion of the FAMEs to fatty acids, the prices of the acids and bases may also contribute to whether or not this process is profitable. Tuning the amount of reactant may be necessary, though this proposed design should be capable of the chemistry ultimately desired.

One important assumption made by this design is that the Omega-3 products ultimately formed and the aqueous products leaving the final acidification step (P3-O) will separate into two phases. This is a good assumption according to the literature, but this assumption is used as the basis to conclude that a perfect separation of Omega-3s from the aqueous components in the exiting stream is attainable (Borhaug et al., 2011). However, because of the other trace chemicals present in the product stream, there is a possibility that a perfect separation is not possible. Performing experiments to identify the partition coefficients of the Omega-3s into these organic solvents would be useful to determine whether the presence of this small amount of organic solvents is sufficient to impact the assumption of two separable phases. In the case that these organics prevent the formation of two phases, an alternative process would have to be designed. Testing the viability of the decanter to separate the Omega-3s cleanly enough to meet market requirements would be crucial if this design were to be implemented.

Another point of future research concerns the selection of the base used in the reaction. Sodium hydroxide was selected because it is cheaper to purchase than potassium hydroxide (Table 11.3). It is worth considering using potassium hydroxide, however, because, with the proper work-up, the muriate of potash (KCl) would be produced in this process and sold as fertilizer to recoup some of the costs associated with the process's design (Baffes, 2018). This would require constructing a wastewater treatment plant capable of removing the organic compounds and precipitating out the salts. This option was not thoroughly considered because the initial investigation into desalination plants revealed the high costs of building a plant, and there were higher costs for desalinating the comparable low volumes of water which this design produces. However, if the demand and price of fertilizer rise high enough, the cost of producing KCl could offset the cost of the desalination plant and might make building a wastewater treatment plant cheaper than shipping it to be processed elsewhere.

The proposed plant shows great promise for the ability to reduce the price of biodiesel. With a growing Omega-3 market around the world, the high demand for the product means that even at the relatively small amounts it will be produced in this plant, the sale revenue is over 100 million dollars a year. This is very promising for the overall proposed process using Yadav and the University of Pennsylvania's work into separation. The next steps for this plant would be additional research and pilot scale studies of the proposed processes to ensure the research used works at larger scales and to invest in the market reports for Omega-3s for a more accurate estimate of their sales revenue. This project ultimately has shown that it can be highly profitable and we recommend investing in the plant's development, but caution that further research into the assumptions made herein is essential before committing to building the plant.

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24. References

Ahuja, K., & Singh, S. (2018, November). Glycerol market size by product type, by source, by application, regional outlook, price trend, competitive market share & forecast 2018-2024. Retrieved from Global Market Insights website: https://www.gminsights.com/industry-analysis/glycerol-market-size

Baffes, J. (2018, November 30). Fertilizer prices to rise in 2019 on supportive fundamentals. Retrieved from http://blogs.worldbank.org/developmenttalk/fertilizer-prices-rise-2019-supportive-fundamentals

Berchmans, H. J., & Hirata, S. (2008). Biodiesel production from crude jatropha curcas L. seed oil with a high content of free fatty acids. *Bioresource Technology*, *99*(6), 1716-1721. Retrieved from ScienceDirect database.

Borhaug, H., Kristensen, M., Brudeli, B., Sontum, P. C., Klaveness, J., & Rongved, P. (2011). Water-soluble omega-3: A concept for purification of fish oil and nutraceuticals? *European Journal of Lipid Science and Technology*, *113*(10), 1235-1242. https://doi.org/10.1002/ejlt.201000502

Chen, T.-C., & Ju, Y.-H. (2001). Polyunsaturated fatty acid concentrates from borage and linseed oil fatty acids. *Journal of the AMerican Oil Chemists' Society*, *78*(5), 485-488. https://doi.org/10.1007/s11746-001-0290-3

Cheong, L.-Z., Guo, Z., Yang, Z., Chua, S.-C., & Xu, X. (2011). Extraction and enrichment of n-3 polyunsaturated fatty acids and ethyl esters through reversible pi-pi complexation with aromatic rings containing ionic liquids [PDF]. *Journal of Agricultural and Food Chemistry*, *59*, 8961-8967.

Commodity market review report. (n.d.). Retrieved from YCharts website: https://ycharts.com/indicators/reports/commodity_markets_review

Crude glycerol. (n.d.). Retrieved from ScienceDirect database.

Department of Energy, Process Design and Economics for the Conversion of Algal Biomass to Hydrocarbons: Whole Algae Hydrothermal Liquefaction and Upgrading, H.R. Rep. No. PNNL-23227 ().

Dolowy, M., & Pyka, A. (n.d.). Chromatographic methods in the separation of long chain mono- and polyunsaturated fatty acids. *Hindawi Publishing Corporation Journal of Chemistry, 2015*.

Dunlop, E. H., Coaldrake, A. K., Silva, C. S., & Seider, W. D. (2013). An energy-limited model of algal biofuel production: Toward the next generation of advanced biofuels. *AiChE, 59*(12), 4641-4655. https://doi.org/10.1002/aic.14251

The Facts on Omega-3 Fatty Acids. (n.d.). Retrieved from WebMD website: https://www.webmd.com/healthy-aging/omega-3-fatty-acids-fact-sheet

Frank, T. C., Dahuron, L., Holden, B. S., Prince, W. D., Seibert, A. F., & Wilson, L. C. (2007). *Liquid liquid extraction and other liquid liquid operations and equipment*. Blacklist, OH: McGraw-Hill Professional Publishing.

Ghebreyessus, K. Y., Schiltz, H., & Angelici, R. J. (2006). Partial separation of polyunsaturated fatty acid esters from fames mixture by adsorption on silver nitrate impregnated silica gels [PDF]. *JAOCS, 83*(7), 645-653.

GOED guidance documents. (2018). In *GOED guidance documents* [PDF].

Goodman, D. S. (1958). The distribution of fatty acids between n-Heptane and aqueous phosphate buffer. *J. Am. Chem. Soc.*, *80*(15), 3887-3892. https://doi.org/10.1021/ja01548a023

Industrial Wastewater Treatment. (n.d.). Retrieved from Clean Harbors website: https://www.cleanharbors.com/services/technical-services/waste-disposal-services/industrial-wastewater-treatment

International energy outlook 2018. (2018, July 24). Retrieved February 27, 2019, from Energy Information Administration website: https://www.eia.gov/outlooks/ieo/

Jacobsen, C., Horne, A. F., Sorenson, A.-D. M., & Nielson, N. S. (Eds.). (2013). *Food enrichment with omega-3 fatty acids*. Retrieved from ProQuest Ebook Central database.

Jimenez, M. J., Esteban, L., Robles, A., Hita, E., Gonzalez, P. A., Munio, M. M., & Molina, E. (2010). Production of triacylglycerols rich in palmitic acid at sn-2 position by lipase-catalyzed acidolysis. *Biochemical Engineering Journal*, *51*(3), 172-179. Retrieved from ScienceDirect database.

Kandula, M. (2018). *U.S. Patent No. WO2018029545*. Washington, DC: U.S. Patent and Trademark Office. Retrieved from https://worldwide.espacenet.com/publicationDetails/biblio?DB=EPODOC&II=0&ND=3&adjacent=true&locale=en_EP&FT=D&date=20180215&CC=WO&NR=2018029545A1&KC=A1

Kywe, T. T., & Oo, M. M. (2009). Production of biodiesel from jatropha oil (Jatropha curcas) in pilot plant. *Proceedings of World Academy of Science, Engineering, and Technology*, *38*, 481-487. Retrieved from

https://www.researchgate.net/publication/242509474_Production_of_Biodiesel_from_Jatropha_Oil_Jatropha_curcas_in_Pilot_Plant

Li, M., Pham, P. J., Wang, T., Pittman, C. U., Jr, & Li, T. (2009). Selective extraction and enrichment of polyunsaturated fatty acid methyl esters from fish oil by novel pi-complexing sorbents. *Separation and Purification Technology*, *66*, 1-8.

Li, X., Zhang, X., Yang, Q., Bao, Z., Ren, Q., Zhang, Z., . . . Yang, Y. (2016). Separation of highly unsaturated fatty acid methyl esters from model bio-oils with ionic liquid cosolvent as extractants. *The Royal Society of Chemistry*, *6*, 60709-60716. https://doi.org/10.1039/c6ra06756e

Ma, F., & Hanna, M. A. (1999). Biodiesel production: A review. *Bioresource Technology*, *70*(1), 1-15. https://doi.org/10.1016/S0960-8524(99)00025-5

Ma, Y., Wang, Z., Yu, C., Yin, Y., & Zhou, G. (2014). Evaluation of the potential of 9 nannochloropsis strains for biodiesel production. *Bioresource Technology*, *167*, 503-509. https://doi.org/10.1016/j.biortech.2014.06.047

Marudhupandi, T., Sathishkumar, R., & Kumar, T. T. A. (2016). Heterotrophic cultivation of nannochloropsis salina for enhancing biomass and lipid production. *Heterotrophic cultivation of Nannochloropsis salina for enhancing biomass and lipid production*, *10*, 8-16. https://doi.org/10.1016/j.btre.2016.02.001

Miazek, K., Kratky, L., Sulc, R., Jirout, T., Aguedo, M., Richel, A., & Goffin, D. (2017). Effect of Organic Solvents on Microalgae Growth, Metabolism and Industrial Bioproduct Extraction: A Review. *Int J Mol Sci*, *18*(7). https://doi.org/10.3390/ijms18071429

Mishra, D. (2018, February 15). The Cost of Desalination. Retrieved from Advisian website: https://www.advisian.com/en-us/global-perspectives/the-cost-of-desalination

Moody, J. W., McGinty, C. M., & Quinn, J. C. (2014). Global evaluation of biofuel potential from microalgae. *PNAS, 111*(23). doi.org/10.1073/pnas.1321652111

Omega-3 fish oil. (n.d.). Retrieved from Jedwards International Inc. website: https://bulknaturaloils.com/omega-3-fish-oil-ee-10-epa-60-dha.html

Omega 3 market size, share, & trends analysis report by application, by region and segment forecasts, 2019-2025. (2019, March). Retrieved from Grand View Research website: https://www.grandviewresearch.com/industry-analysis/omega-3-market?utm_source=google&utm_medium=cpc&utm_campaign=AdWords_Omega3_CMFE&gclid=EAIaIQobChMI4t_Zp6nQ4QIVxF6GCh3vXQEAEAAYASAAEgI2dfD_BwE

Pando, M. E., Rodríguez, A., Galdames, A., Berríos, M. M., Rivera, M., Romero, N., . . . Aubourg, S. P. (2018). Maximization of the docosahexaenoic and eicosapentaenoic acids content in concentrates obtained from a by-product of rainbow trout (Oncorhynchus mykiss) processing. *European Food Research and Technology*, *244*(5). https://doi.org/10.1007/s00217-017-3013-0

Potassium chloride. (n.d.). Retrieved from Crop Nutrition website: https://www.cropnutrition.com/potassium-chloride

Rahmat, B., Setiasih, I. S., & Kastaman, R. (2013). Biodiesel reactor design with glycerol separation to increase biodiesel production yield. *Makara Seri Teknologi, 17,* 11-16.

Salimon, J., Abdullah, B. M., & Salih, N. (2011). Hydrolysis optimization and characterization study of preparing fatty acids from jatropha curcasseed oil. *Chemistry Central Journal*, *5*(67). Retrieved from BMC Chemistry database.

Sangster, J. (1989). Octanol-Water partition coefficients of simple organic compounds. *Journal of Physical and Chemical Reference Data*, *18*(3), 1111-1227. https://doi.org/10.1063/1.555833

Seider, W. D., Lewin, D. R., Seader, J. D., Widagdo, S., Gani, R., & Ng, K. M. (2017). *Product and process design principles: Synthesis, analysis and evaluation* (4th ed.). Wiley.

Silva, C., Soh, L., Barberio, A., Zimmerman, J., & Seider, W. D. (2016). Phase equilibria of triolein to biodiesel reactor systems. *Fluid Phase Equilibria*, *409*, 171-192. Retrieved from ScienceDirect database.

Silva, C. J. (2015). *Commercial- scale conversion of algae to biofuel* (Unpublished doctoral dissertation). U of Pennsylvania.

Simpson, R. B., Ashbrook, J. D., Santos, E. C., & Spector, A. A. (1974). Partition of fatty acids. *Journal of Lipid Chemistry*, *15*, 415-422. Retrieved from http://www.jlr.org/content/15/4/415.full.pdf

Sodium hydroxide solution. (n.d.). Retrieved from Alibaba website: https://www.alibaba.com/product-detail/Sodium-Hydroxide-Solution-50-NaOH-Caustic_60485628232.html?spm=a2700.7724857.normalList.30.3654b6311lYOrs

Soh, L., Chen, C. C., Kwan, T. A., & Zimmerman, J. B. (2011). Role of co2 in mass transfer, reaction kinetics, and interphase partitioning for the transesterification of triolein in an expanded methanol system with heterogenous acid catalyst. *ACS Sustainable Chemical Engineering*, *3*(11), 2669-2677. https://doi.org/10.1021/acssuschemeng.5b00472

Soh, L., Curry, J., Beckman, E. J., & Zimmerman, J. B. (2014). Effect of system conditions for biodiesel production via transesterification using carbon dioxide-methanol mixtures in

the presence of a heterogenous catlyst. *ACS Sustainable Chemical Engineering*, *2*(3), 387-395. https://doi.org/10.1021/sc400349g

Soh, L., & Zimmerman, J. (2011). Biodiesel production: The potential of algal lipids extracted with supercritical carbon diozide [PDF]. *Green Chemistry*, *13*, 1422-1429.

Statistical review of world energy. (n.d.). Retrieved February 27, 2019, from BP website: https://www.bp.com/en/global/corporate/energy-economics/statistical-review-of-world-energy.html

Swanson, D., Block, R., & Mousa, S. A. (2012). Omega-3 Fatty Acids EPA and DHA: Health Benefits Throughout Life. Advances in Nutrition, 3(1), 1-7. doi.org/ 10.3945/an.111.000893

Teramoto, M., Matsuyama, H., Ohnishi, N., Uwagawa, S., & Nakai, K. (1994). Extraction of ethyl and methyl esters of polyunsaturated fatty acids with aqueous silver nitrate solutions. *Industrial and Engineering Chemistry Research*, *33*, 341-345.

2019 refinement to the 2006 IPCC guidelines for national greenhouse gas inventories. (2017, December 4). Retrieved February 27, 2019, from IPCC website: https://www.ipcc.ch/report/2019-refinement-to-the-2006-ipcc-guidelines-for-national-greenhouse-gas-inventories/

Wholemega. (n.d.). Retrieved from Whole Foods Market website: https://www.wholefoodsmarket.com/products/wholemega

Why is the Ocean Salty? (n.d.). Retrieved from USGS website: https://www.usgs.gov/special-topic/water-science-school/science/why-ocean-salty?qt-science_center_objects=0#qt-science_center_objects

Xing, H., Zhang, X., Yang, Q., Liu, R., Bao, Z., Su, B., . . . Ren, Q. (2014). Separation of long chain fatty acids with different number of unsaturated bonds by fractional extraction: Experimental and cosmo-rs study. *Food Chemistry*, *143*, 411-417. Retrieved from Elsevier database.

Yadav, G., Fabiano, L. A., Seider, W. D., Soh, L., & Julie Zimmerman. (2018). *Process intensification of algae oil extraction to biodiesel - RAPID research needs plus alternatives*. Unpublished working paper, U of Pennsylvania, Lafayette U, Yale U.

25. Appendix

25.1 Project Problem Sheet

11. Conversion of Omega-3 Fatty Acids from Algae Biomass to Biodiesel (Recommended by Leonard A. Fabiano, Geetanjali Yadav, and Warren D. Seider, UPenn)

After extraction of triglyceride oil from microalgae, Zhu et al. (2017) designed a plant to produce omega-3 fatty acids, which provide significant health benefits, improving heart and mental health. Then, a new intensified process to produce commodity quantities of biodiesel from microalgae (Yadav et al., 2018), especially used as transportation fuel, also produced omega-3 fatty acids as a co-product, which are useful as infant food and animal feed. Moreover, because excess quantities of omega-3 fatty acids are produced, they can be converted to biodiesel fuel via a reaction path that uses ultrasonic energy for the transesterification process (Armenta et al. 2007). This way, a biorefinery is established from CO_2 sequestered algal biomass to produce fuel, feed, and nutraceuticals using an intensified process.

The hydrothermal liquefaction (HTL) process (Biddy et al., 2013; Anderson, 2013), designed by the DOE Pacific Northwest National Laboratory (PNNL), operates at temperatures (350°C) and pressures (200 bar) too high to produce health supplements. A key advantage is that 65 wt% of the algae carbon is converted to transportation fuels. But, the intensified process (Yadav et al., 2018), because it operates at just 90°C and much lower pressures, introduces a new flexibility to produce quantities of omega-3 fatty acids as co- products of the main biodiesel fuel product. The remainder can be converted to biodiesel using the Armenta et al. (2007) transesterification.

As microalgae species contain different types of triglycerides (carbon chain-length and saturation), different kinds of products may be expected from the same strain depending on various process and culture conditions (Vazhappilly and Chen, 1998). This design project involves adjusting and improving (replacing the ball mills and hexane extraction with microbubble extraction) in the Zhu et al. (2017) plant and, for adjustable quantities of residual algae biomass, designing a plant using the Armenta et al. (2007) transesterification. The intent is to design a plant that provides the flexibility to adjust, within limits, the amount of residual algae biomass to be transesterified, depending on consumer demand for the bio(co)products. Given the relatively high prices of omega-3 fatty acids and animal feeds, a key question involves whether the combined processes produce biofuels, and these bio(co)products, less expensively than the HTL process. If so, it will be recommended that a pilot-plant design be undertaken to demonstrate the feasibility of these combined processes.

Stated differently, the student design team will decide upon the size of the plant and the coproduct slate to maximize the economic viability of the project, while allowing flexibility for adjusting the product slate depending on then-current customer demand (prices).

References

Zhu, A., L. Nowack, and M.-Y. Jeong, *On the Production of High-Purity Docosa-hexaenoic Acid from Heterotrophic Microalgae*, Univ. of Pennsylvania Library (2017): http://repositoryupenn.edu/cbe_sdr

Yadav, G., L. A. Fabiano, W. D. Seider, L. Soh, and J. Zimmerman, "Process intensification of algae oil

extraction to biodiesel," in Ed., M. R. Eden, M. Ierapetritou, G. P. Towler, *Proceedings of the 13th Int'l. Symp. on PSE,* San Diego, CA (2018).

Armenta, R. E., M. Vinatoru, A. M. Burga, J. A. Kralovec, and C. J. Barrou, "Transesterification of fish oil to produce fatty acid ethyl esters using ultrasonic energy," *J. Amer. Oil Chem. Soc.*, **84**, 1035-1052 (2007).

Biddy, M., R. Davis, S. Jones, and Y. Zhu, *Whole Algae Hydrothermal Liquefaction Technology Pathway*, Technical Report NREL/TP-5100-58051, PNNL-22314, March 2013. Available from: https://www.osti.gov/biblio/1076659-whole-algae-hydrothermal-liquefaction-technology-pathway

Anderson, T., Algae to crude oil: Million-year natural process takes minutes in the lab, Dec. 19, 2013. Obtain news article from W. D. Seider.

Vazhappilly, R., and F. Chen, "Eicosapentaenoic acid and docosahexaenoic acid production potential of microalgae and their heterotrophic growth," *J. Amer. Oil Chem. Soc.*, **75**, 3, 393-397 (1998).

25.2 Sample Calculations

25.2.1 FAME Composition Calculations

Fatty Acid	N. salina CCMP537		N. salina CCMP1176		Heterotrophic		Photoautotrophic	
12 0	–	0	–	0	2.80 ± 0.037	2.8	1.3 ± 0.002	1.3
14 0	3.34 ± 0.19	3.34	2.08 ± 0.31	2.08	8.01 ± 0.009	8.01	5.9 ± 0.01	5.9
14 1	–	0	–	0	1.75 ± 0.01	1.75	2.7 ± 0.023	2.7
16 0	32.23 ± 0.67	32.23	32.04 ± 1.80	32.04	22.84 ± 0.265	22.84	40.7 ± 0.55	40.7
16 1	25.41 ± 0.82	25.41	29.94 ± 0.85	29.94	4.71 ± 0.005	4.71	8.6 ± 0.36	8.6
16 2	2.98 ± 0.95	2.98	–	0	–	0	–	0
18 0	2.47 ± 0.70	2.47	3.19 ± 0.18	3.19	2.01 ± 0.005	2.01	0.78 ± 0.001	0.78
18 1	15.46 ± 0.71	15.46	9.37 ± 0.15	9.37	4.65 ± 0.028		5.5 ± 0.15	
18 1 n-9	–	0	–	0	3.92 ± 0.01	8.57	4.9 ± 0.03	10.4
18 2	2.89 ± 0.29	2.89	2.58 ± 0.40	2.58	3.65 ± 0.21	3.65	1.87 ± 0.03	1.87
18 3	0.65 ± 0.04	0.65	0.90 ± 0.06	0.9	0.58 ± 0.56	0.58	0.3 ± 0.001	0.3
18 4	–	0	–	0	1.62 ± 0.19	1.62	2.37 ± 0.026	2.37
20 0	–	0	–	0	1.48 ± 0.015	1.48	0.3 ± 0.001	0.3
20 1 n-11	–	0	–	0	2.86 ± 0.007	2.86	1.83 ± 0.02	1.83
20 1 n-9	–	0	–	0	1.32 ± 0.015	1.32	0.26 ± 0.001	0.26
20 4	3.64 ± 0.07	3.64	7.16 ± 0.75	7.16	–	0	–	0
20 5	10.93 ± 0.14	10.93	12.74 ± 1.84	12.74	30.54 ± 1.19	30.54	17.4 ± 0.62	17.4
22 0	–	0	–	0	0.86 ± 0.002	0.86	0.48 ± 0.002	0.48
22 1	–	0	–	0	0.72 ± 0.004	0.72	0.43 ± 0.008	0.43
22 6	–	0	–	0	2.6 ± 0.04	2.6	1.9 ± 0.007	1.9
24 0	–	0	–	0	1.41 ± 0.173	1.41	1.16 ± 0.005	1.16
24 1	–	0	–	0	1.67 ± 0.027	1.67	1.32 ± 0.017	1.32
SFA	38.04 ± 1.81	38.04	37.31 ± 2.29	37.31	39.41 ± 0.506	39.41	50.62 ± 0.571	50.62
MUFA	40.87 ± 1.53	40.87	39.31 ± 1.00	39.31	21.6 ± 0.106	21.6	25.54 ± 0.60	25.54
PUFA	18.11 ± 0.54	21.09	23.38 ± 3.05	23.38	38.99 ± 2.19	38.99	23.84 ± 0.68	23.84
UFA	58.98 ± 2.07	61.96	62.69 ± 4.05	62.69		60.59		49.38

Fatty Acid	Average	Label	Calculation
12 0	1.025	Minor	
14 0	4.8325	SFA Etc	7.28
14 1	1.1125	Minor	
16 0	31.9525	SFA	31.9525
16 1	17.165	MUFA	17.165
16 2	0.745	Minor	
18 0	2.1125	SFA	2.1125
18 1	10.95	MUFA Etc	14.665
18 2	2.7475	PUFA Etc	7.7975
18 3	0.6075	Minor	
18 4	0.9975	Minor	
20 0	0.445	Minor	
20 1 n-11	1.1725	Minor	
20 1 n-9	0.395	Minor	
20 4	2.7	Minor	
20 5	17.9025	EPA	17.9025
22 0	0.335	Minor	
22 1	0.2875	Minor	
22 6	1.125	DHA	1.125
24 0	0.6425	Minor	
24 1	0.7475	Minor	
SFA	41.345		41.345
MUFA	31.83		31.83
PUFA	26.825		26.825
UFA	58.655		58.655

25.2.2 Profitability Spreadsheet Calculations

Table 25.2.1 Equipment Cost Inputs for Profitability

Equipment Costs				
Equipment Description	**Type**	**Purchase Cost**	**Bare Module Factor**	**Bare Module Cost**
Name	(must be filled-in!)		(default 3.21 if blank)	
Clean FAME to Splitter Pump	Process Machinery	$5,230	3.30	$17,259
To LLE pump	Process Machinery	$4,695	3.30	$15,494
LLE to LLE pump	Process Machinery	$5,275	3.30	$17,408
Product FAME pump	Process Machinery	$5,057	3.30	$16,688
Silver Pump	Process Machinery	$5,808	3.30	$19,166
Hexene Pump	Process Machinery	$5,808	3.30	$19,166
Decanter	Process Machinery	$51,139	4.16	$212,738
FAME Flash	Process Machinery	$51,895	4.16	$215,883
Glycerol Sererator	Process Machinery	$24,659	4.16	$102,581
Hexene sep	Process Machinery	$21,108	4.16	$87,809
LLE 1	Process Machinery	$48,668	4.16	$202,459
LLE 2	Process Machinery	$33,523	4.16	$139,456
BASEREAC (2)	Process Machinery	$56,550	4.16	$235,249
ACIDREAC (2)	Process Machinery	$41,298	4.16	$171,798
DIST-Reflux Accumulator	Process Machinery	$15,783	4.16	$65,659
DECANT	Process Machinery	$29,785	4.16	$123,904
BASEREAC Jacket (2)	Process Machinery	$34,750	4.16	$144,560
ACIDREAC Jacket (2)	Process Machinery	$23,712	4.16	$98,642
BASEREAC Agitator (2)	Process Machinery	$24,376	3.30	$80,441
ACIDREAC Agitator (2)	Process Machinery	$15,121	3.30	$49,900
P-DIST	Process Machinery	$12,505	3.30	$41,267
P-Reflux	Process Machinery	$6,017	3.30	$19,857
P-LLE	Process Machinery	$10,756	3.30	$35,495
P-BASE	Process Machinery	$156,314	1.00	$156,314
P-ACID	Process Machinery	$109,417	1.00	$109,417
DIST-Cond	Process Machinery	$11,293	3.17	$35,798
DIST-Reboiler	Process Machinery	$53,090	3.17	$168,297
HX-MEOH	Process Machinery	$12,048	3.17	$38,192
DIST	Process Machinery	$93,810	4.16	$390,249
silver nitrate	Catalysts	1700180.587	1.00	$1,700,181
1- hexene	Catalysts	4640.934428	1.00	$4,641
methanol for lle	Catalysts	2140.263829	1.00	$2,140
methanol for reactor	Catalysts	375.5350893	1.00	$376
Nitrogen	Catalysts	$298,490	1.00	$298,490
Omega-3 Product	Storage	$217,475	4.00	$869,899
Neutral Wastewater	Storage	$215,762	4.00	$863,048
NaOH Solution	Storage	$56,572	4.00	$226,287
HCl Solution	Storage	$54,305	4.00	$217,222
Total				***7,213,428***

Variable Cost Summary

Variable Costs at 100% Capacity:

General Expenses

Selling / Transfer Expenses:		$	12,076,690
Direct Research:		$	19,322,703
Allocated Research:		$	2,012,782
Administrative Expense:		$	8,051,126
Management Incentive Compensation:		$	5,031,954
Total General Expenses		$	46,495,255
Raw Materials	$0.934225 per kg of Biodiesel		$464,294,192
Byproducts	$0.244511 per kg of Biodiesel		($121,518,019)
Utilities	$0.010019 per kg of Biodiesel		$4,979,354
Total Variable Costs		**$**	**394,250,782**

Fixed Cost Summary

Operations

Direct Wages and Benefits	$	1,081,600
Direct Salaries and Benefits	$	162,240
Operating Supplies and Services	$	64,896
Technical Assistance to Manufacturing	$	780,000
Control Laboratory	$	845,000
Total Operations	**$**	**2,933,736**

Maintenance

Wages and Benefits	$	421,336
Salaries and Benefits	$	105,334
Materials and Services	$	421,336
Maintenance Overhead	$	21,067
Total Maintenance	**$**	**969,074**

Operating Overhead

General Plant Overhead:	$	125,706
Mechanical Department Services:	$	42,492
Employee Relations Department:	$	104,460
Business Services:	$	131,018
Total Operating Overhead	**$**	**403,676**

Property Taxes and Insurance

Property Taxes and Insurance:	$	187,261

Other Annual Expenses

Rental Fees (Office and Laboratory Space):	$	-
Licensing Fees:	$	-
Miscellaneous:	$	-
Total Other Annual Expenses	**$**	**-**
Total Fixed Costs	**$**	**4,493,747**

Investment Summary

Total Bare Module Costs:			
Fabricated Equipment	$	-	
Process Machinery	$	3,031,145	
Spares	$	-	
Storage	$	2,176,456	
Other Equipment	$	-	
Catalysts	$	2,005,827	
Computers, Software, Etc.	$	-	
Total Bare Module Costs:			**$ 7,213,428**
Direct Permanent Investment			
Cost of Site Preparations:	$	360,671	
Cost of Service Facilities:	$	360,671	
Allocated Costs for utility plants and related facilities:	$	-	
Direct Permanent Investment			**$ 7,934,771**
Total Depreciable Capital			
Cost of Contingencies & Contractor Fees	$	1,428,259	
Total Depreciable Capital			**$ 9,363,030**
Total Permanent Investment			
Cost of Land:	$	187,261	
Cost of Royalties:	$	-	
Cost of Plant Start-Up:	$	936,303	
Total Permanent Investment - Unadjusted			$ 10,486,594
Site Factor			1.00
Total Permanent Investment			**$ 10,486,594**

Working Capital

		2021		2022		2023
Accounts Receivable	$	14,889,069	$	7,444,535	$	7,444,535
Cash Reserves	$	350,375	$	175,187	$	175,187
Accounts Payable	$	(17,356,693)	$	(8,678,346)	$	(8,678,346)
Biodiesel Inventory	$	1,985,209	$	992,605	$	992,605
Raw Materials	$	1,144,835	$	572,417	$	572,417
Total	**$**	**1,012,796**	**$**	**506,398**	**$**	**506,398**
Present Value at 15%	*$*	*880,692*	*$*	*382,910*	*$*	*332,965*

Total Capital Investment		**$ 12,083,160**

Profitability Measures

The Internal Rate of Return (IRR) for this project is 15.08%

The Net Present Value (NPV) of this project in 2020 is $ 56,900

ROI Analysis (Third Production Year)

Annual Sales	**362,300,689**
Annual Costs	**(359,319,450)**
Depreciation	**(838,927)**
Income Tax	**(492,732)**
Net Earnings	**1,649,580**
Total Capital Investment	**12,512,185**
ROI	**13.18%**

Sensitivity Analyses

Note: The Sensitivity Analyses section below takes quite a bit of memory to update each time a cell is changed; therefore, automatic calculations are turned off. After making your axis selections, press "F9" to recalculate the IRR values. (These two lines may be deleted before printing.)

	Vary Initial Value by +/-
x-axis	5%
y-axis	10%

						Variable Costs					
	$374,538,243	$378,480,750	$382,423,258	$386,365,766	$390,308,274	***$394,250,782***	$398,193,290	$402,135,797	$406,078,305	$410,020,813	$413,963,321
$0.73	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.75	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.76	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.78	33.23%	14.69%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.79	63.23%	48.43%	32.73%	14.89%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.81	89.24%	75.74%	61.88%	47.50%	32.27%	15.08%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$0.83	112.84%	100.15%	87.26%	74.11%	60.61%	46.62%	31.84%	15.25%	-14.75%	Negative IRR	Negative IRR
$0.84	134.68%	122.57%	110.34%	97.96%	85.38%	72.56%	59.41%	45.80%	31.43%	15.41%	-10.59%
$0.86	155.10%	143.45%	131.73%	119.90%	107.96%	95.87%	83.60%	71.10%	58.28%	45.01%	31.05%
$0.87	174.31%	163.06%	151.74%	140.37%	128.91%	117.36%	105.70%	93.89%	81.91%	69.71%	57.20%
$0.89	192.47%	181.56%	170.60%	159.60%	148.55%	137.43%	126.23%	114.94%	103.54%	92.01%	80.30%

Product Price

25.2.3 Liquid- Liquid Extraction Calculations

$$L_0 + V_2 = L_1 + V_1 = M \quad [1]$$

$$L_0 x_{A0} + V_2 y_{A2} = L_1 x_{A1} + V_1 y_{A1} = M x_{AM} \quad [2]$$

$$L_0 x_{C0} + V_2 y_{C2} = L_1 x_{C1} + V_1 y_{C1} = M x_{CM} \quad [3]$$

where

L_i = the molar flowrate of heavier phase out of stage i

V_i = the molar flowrate of lighter phase out of stage i

M = the total molar flow rate into or out of the unit

x_{ij} = the mol fraction of component i leaving stage j in the L phase

y_{ij} = the mol fraction of component i leaving stage j in the V phase

x_{iM} = the mol fraction of component i

$$y_{A1} = K x_{A1} \quad [4]$$

$$K = \frac{mol\ fraction\ of\ solute\ in\ extract}{mol\ fraction\ of\ solute\ in\ raffinate} \quad [5]$$

$$E = \frac{KL}{V} \quad [6]$$

$$N = \frac{ln\left(\frac{x_0 - \frac{y_{N+1}}{K}}{x_N - \frac{y_{N+1}}{K}} \times (1-E) + E\right)}{ln\left(\frac{1}{E}\right)} \quad [7]$$

N = number of theoretical stages

x_0 = mole fraction of solute in the feed (L_0) to the process

x_N = mole fraction of solute in the raffinate (L_N) leaving the process

y_{N+1} = mole fraction of solute in the solvent (V_{N+1}) entering the process

E = extraction factor

Mass Balance Calculations:

Goal: 1440 kg/hr= 4347.97 mol/hr

Silver Nitrate Required:

$$EPA * 5 + DHA * 6 = 25021.79 \frac{mol}{hr} Silver\ ion\ required$$

$$25021.79 \frac{mol}{hr} * \frac{dm^3}{4\ mol} * \frac{.001 m^3}{1\ dm^3} * \frac{792\ kg}{m^3} = 9204.77\ \frac{kg}{hr}\ Silver\ Nitrate\ Solution$$

$$Methanol\ Required = 9204.77 - (25021.79 \frac{mol\ Ag}{hr} * 169.87 \frac{g}{mol} * \frac{1\ kg}{1000 g} = 4954.32\ \text{kg/hr}$$

1-Hexene Required:

Expect recovery from Ag to be 88% and maximum mass fraction in 1-hexene solution to be .45

$$Hexene = \frac{1440 \frac{kg}{hr}}{.45} = \frac{3200.65\ kg}{hr}$$

Mass Balance on Methyl EPA and Methyl DHA in LLE Columns

	Methyl EPA		Methyl DHA	
EPA DHA Balance	LLE 1	LLE 2	LLE 1	LLE 2
Inlet Aqueous	**Silver Solution**	**Complexed Silver**	**Silver Solution**	**Complexed Silver**
mass kg/hr	0	1518.551843	0	103.39635
mol /hr free Ag	0	4606.609313	0	289.7550216
Inlet Organic	**FAMEs**	**1- hexene**	**FAMEs**	**1- hexene**
mass kg/hr	1533.89075	0	104.4407576	0
mol /hr	4653.14072	0	292.68184	0
Outlet Aqueous	**Complexed Silver**	**Recycled Silver**	**Complexed Silve**	**Recycled Silver**
mass kg/hr	1518.551843	170.0778064	103.39635	11.5803912
mol /hr	4606.609313	515.940243	289.7550216	32.45256242
Outlet Organic	**Light FAMEs**	**Omega 3s in Hexene**	**Light FAMEs**	**Omega 3s in Hexene**
mass kg/hr	15.3389075	1348.474036	0	91.81595882
mol /hr	46.5314072	4090.66907	0	257.3024592
		Output to Reaction	1440.289995	kg/hr

Mass Balance Calculations for LLEs

	LLE 1	LLE 2
Inlet Aqueous	**Ag in Methanol**	**Ag complex in methanol**
mass kg/hr	9204.767594	10644.76759
mol /hr free Ag necessary	25021.79464	
mol/hr solution	179650.834	184547.1983
mass frac epa dha	0	0.152370465
mol frac epa dha	0	0.026531773
Inlet Organic	**FAMEs**	**1- hexene**
mass kg/hr	7625	3200.644433
mol /hr	26344	38030.10942
mass frac epa	0.201166	0
mass frac dha	0.013697149	0
mol frac dha	0.01111	0
mol frac epa	0.17663	0
Outlet Aqueous	**Ag complex in methanol**	**Recyclable Ag in CH4OH**
mass kg/hr	10644.76759	9204.477599
mol /hr	184547.1983	180199.2268
mass frac epa dha	0.152370465	0.019735851
mol frac epa dha	0.026531773	0.003043258
Outlet Organic	**Light FAMEs**	**epa dha in hexene**
mass kg/hr	6185	4640.934428
mol /hr	21447.63567	42378.08095
mass frac epa dha	0.002480017	0.45
mol frac epa dha	0.002169536	0.102599538
Stages Calc		
k	0.122	1.04
E	0.141085762	0.899282828
N	2.1954047	4.869437969
efficiency	0.25	0.25
trays for column	9	20
RTD (minutes)	25	10
Volume L l/min	137.507	79.26311127
Volume V l/min	190.1025938	219.8423708
Volume of Column liter	8190.239846	2991.054821
h value	6.229561015	5.738905247
Diameter ft	6	4
Radius	3	2
Height ft	12.22956101	9.738905247
Height Rounded	12.3	9.8

25.2.4 Water Jacket Calculations

BASEREAC						
Q	-8876.18	cal/s		Note: use regular cooling water		
	-37.1379	kW				
	-126720	BTU/hr				
U	200	Btu/(◦F - ft2 - hr)				
T h, in	161.4487	°F	71.91593	C		
T h, out	149	°F	65	C		
T c, in	90	°F	32.22222	C		
T c, out	120	°F	48.88889	C		
del T cw	30	°F				
del T rct	12.44868	°F				
R	0.414956					
S	0.419882					
del T lm	19.95414					
Q = UA(dTlm)						
A	31.75277	ft^2	(minimum surface area required)			
BASEREAC SA: (surface area available)						
D	H	R	SA [ft2]			
4	13	2	163.3628	[2*pi*R*H]		
Q = mc(dT)						
(dT)	16.66667					
c	1	cal/g/K				
[g/s]	532.5706					
[mol/hr]	106425.4					
[kg/hr]	1917.254					

ACIDREAC								
Q	-42223.5	cal/s		Note: Need to use chilled water				
	-176.663	kW						
	-602799	BTU/hr		(Used Q for 2 reactors)				
U	200	Btu/(◦F - ft2 - hr)		Note: Table 12.5 (Jacket-Water, Water-Water)				
T h, in	165.1461	°F	73.97008	C				
T h, out	77	°F						
T c, in	45	°F	7.222222	C				
T c, out	90	°F	32.22222	C				
del T cw	45	°F						
del T rct	88.14614	°F						
R	1.958803							
S	0.374544							
del T lm	64.17371							
Q = UA(dTlm)								
A	46.9662	ft^2	(minimum surface area required)					
ACIDREAC SA: (surface area available)								
D	H	R	SA [ft2]					
3	10	1.5	94.24778	[2*pi*R*H]				
Q = mc(dT)								
(dT)	25							
c	1	cal/g/K						
[g/s]	1688.938							
[mol/hr]	337506.4							
[kg/hr]	6080.178							

25.5.5 Wastewater Treatment Calculations

1: Dilution with process water, recycle to algae					
	Need salinity = 3.5 g NaCl/kg water				
	Na+ [g/hr]	135074.7			
	Cl- [g/hr]	208308			
	NaCL [g/hr]	343382.8			
	Already present				
	Water [kg/hr]	1511.929			
	Required [kg/hr]	98109.36			
	To purchase	[kg/hr]	[L/hr]	[gal/hr]	[gal/yr]
		96597.43	96597.42855	25518.34	2.01E+08
	Table 17.1	Process Water: $0.80/1000 gal			
	[gal/hr]	25518.34		[$/hr]	20.41467
	[gal/yr]	2.01E+08		[$/yr]	160949.3
	Methanol [g/hr]	5071.014			
	Water Volume [L/hr]	98109.36			
	Methanol Conc [g/L]	0.051687			
2: Send to water treatment plant					
	Table 17.1: Wastewater treatment: $0.15/lb organic removed				
	Organics				
	Methanol [lb/hr]	11.17967			
	1-Hexene [lb/hr]	0.234741			
	Total [lb/hr]	11.41441		[$/hr]	1.712162
	Total [lb/yr]	89991.23		[$/yr]	13498.68

25.5.6 Storage Tank and Feedstock Calculations

Omega-3 Product			
Storage Tank			
	Volume [L/hr]	1669.736	(Aspen)
	Vol [L/day]	40073.66	
	Tank Capacity [L]	420773.4	[7 days]
	Tank Capacity [gal]	111156.6	

Neutral Wastewater			
Storage Tank			
	Volume [L/hr]	1644.198	
	Vol [L/day]	39460.75	
	Tank Capacity [L]	414337.9	[7 days]
	Tank Capacity [gal]	109456.5	

NaOH	NaOH Reaction						
		MW	[mol/hr]	[kg/hr]	wt%		
	NaOH	39.997	5425.944922	217.0215	0.5		
	Water	18.015	12046.71213	217.0215	0.5		
	Total			434.043			
		KOH (50 wt%): $300/metric ton					
	[kg/hr]	434.043					
	[metric ton/hr]	0.434043		[$/hr]	130.2129		
	[metric ton/yr]	3421.995		[$/yr]	1026599		
Water		MW	[mol/hr]	[kg/hr]	[L/hr]	[gal/hr]	[gal/yr]
	Process	18.015	45080.50066	812.1252			
	To Purchase		33033.78853	595.1037	595.1037	157.2098	1239441.8
	Table 17.1	Process Water: $0.80/1000 gal					
	[gal/hr]	157.2098		[$/hr]	0.125768		
	[gal/yr]	1239442		[$/yr]	991.5534		
Storage Tank							
	Volume [L/hr]	846.7716					
	Vol [L/day]	20322.52					
	Tank Capacity [L]	30483.78	[1 day]				
	Tank Capacity [gal]	8052.962					

NaOH	NaOH Water Treatment						
		MW	[mol/hr]	[kg/hr]	wt%		
	H+ Present		449.6239184	0.453073			
	NaOH	39.997	449.6239184	17.98361	0.5		
	Water	18.015	998.2574446	17.98361	0.5		
	Total			35.96722			
		KOH (50 wt%): $300/metric ton					
	[kg/hr]	35.96722					
	[metric ton/hr]	0.035967		[$/hr]	10.79016		
	[metric ton/yr]	283.5655		[$/yr]	85069.66		

HCl	HCl Reaction						
		MW	[mol/hr]	[kg/hr]	wt%		
	HCl	36.46	5875.568845	214.2232	0.3		
	Water	18.015	27746.55714	499.8542	0.7		
				714.0775			
		HCl (30 wt%): $100/metric ton					
	[kg/hr]	714.0775					
	[metric ton/hr]	0.714077		[$/hr]	71.40775		
	[metric ton/yr]	5629.787		[$/yr]	562978.7		
Water		MW	[mol/hr]	[kg/hr]	[L/hr]	[gal/hr]	[gal/yr]
	Process	18.015	36514.19354	657.8032			
	To Purchase		8767.636397	157.949	157.949	41.7257	328965.45
	Table 17.1	Process Water: $0.80/1000 gal					
	[gal/hr]	41.7257		[$/hr]	0.033381		
	[gal/yr]	328965.4		[$/yr]	263.1724		
Storage Tank							
	Volume [L/hr]	781.907					
	Vol [L/day]	18765.77					
	Tank Capacity [L]	28148.65	[1 day]				
	Tank Capacity [gal]	7436.087					

25.3 MSDS Sheets

SAFETY DATA SHEET

Version 5.3
Revision Date 05/23/2016
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 1-Hexene

Product Number : 240761
Brand : Aldrich

CAS-No. : 592-41-6

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 2), H225
Aspiration hazard (Category 1), H304

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)
H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P280 Wear protective gloves/ eye protection/ face protection.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated

	clothing. Rinse skin with water/ shower.
P331	Do NOT induce vomiting.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula	:	$C_6H_{12}C_6H_{12}$
Molecular weight	:	84.16 g/mol
CAS-No.	:	592-41-6
EC-No.	:	209-753-1

Hazardous components

Component	Classification	Concentration
Hex-1-ene		
	Flam. Liq. 2; Asp. Tox. 1; H225, H304	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): Flammable liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Hex-1-ene	592-41-6	TWA	50.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment		
		TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment		
		PEL	50 ppm 180 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 30 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	-140.0 °C (-220.0 °F)
f)	Initial boiling point and boiling range	60 - 66 °C (140 - 151 °F) - lit.
g)	Flash point	-25.0 °C (-13.0 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Lower explosion limit: 1.2 %(V)
k)	Vapour pressure	413.3 hPa (310.0 mmHg) at 37.7 °C (99.9 °F) 206.6 hPa (155.0 mmHg) at 21.1 °C (70.0 °F)

l)	Vapour density	No data available
m)	Relative density	0.678 g/cm3 at 25 °C (77 °F)
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	253.0 °C (487.4 °F)
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information
No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
acids, Oxidizing agents

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
No data available

LC50 Inhalation - Rat - 4.0 h - 32000. ppm
Remarks: Behavioral:General anesthetic. Behavioral:Somnolence (general depressed activity). Lungs, Thorax, or Respiration:Other changes.

Dermal: No data available

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
May be fatal if swallowed and enters airways.The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

Additional Information
RTECS: MP6670000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, May cause cyanosis.

Central nervous system -

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2370 Class: 3 Packing group: II
Proper shipping name: 1-Hexene

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG
UN number: 2370 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: 1-HEXENE

IATA
UN number: 2370 Class: 3 Packing group: II
Proper shipping name: 1-Hexene

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

	CAS-No.	Revision Date
Hex-1-ene	592-41-6	2007-03-01

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Asp. Tox.	Aspiration hazard
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.

HMIS Rating
Health hazard: 0
Chronic Health Hazard:

Flammability:	3
Physical Hazard	0

NFPA Rating

Health hazard:	0
Fire Hazard:	3
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.3 Revision Date: 05/23/2016 Print Date: 11/10/2018

SAFETY DATA SHEET

Version 5.7
Revision Date 02/02/2018
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Diethyl ether

Product Number : 472484
Brand : Sigma-Aldrich
Index-No. : 603-022-00-4

CAS-No. : 60-29-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 1), H224
Acute toxicity, Oral (Category 4), H302
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)
H224 Extremely flammable liquid and vapour.
H302 Harmful if swallowed.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use only non-sparking tools.

P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash 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 protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P312	Call a POISON CENTER/doctor if you feel unwell.
P330	Rinse mouth.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

May form explosive peroxides., Repeated exposure may cause skin dryness or cracking.
May form explosive peroxides.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Ether Ethyl ether
Formula	:	$C_4H_{10}O$
Molecular weight	:	74.12 g/mol
CAS-No.	:	60-29-7
EC-No.	:	200-467-2
Index-No.	:	603-022-00-4
Registration number	:	01-2119535785-29-XXXX

Hazardous components

Component	Classification	Concentration
Diethyl ether		
	Flam. Liq. 1; Acute Tox. 4; STOT SE 3; H224, H302, H336	90 - 100 %
Ethanol		
	Flam. Liq. 2; Eye Irrit. 2A; H225, H319	1 - 5 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Diethyl ether	60-29-7	TWA	400.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	500.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		See Appendix D - Substances with No Established RELs		
		TWA	400.000000 ppm 1,200.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		See Appendix D - Substances with No Established RELs		
		TWA	400 ppm 1,200 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	400 ppm 1,200 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	500 ppm 1,500 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	400 ppm 1,200 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	500 ppm 1,500 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
Ethanol	64-17-5	TWA	1,000.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Confirmed animal carcinogen with unknown relevance to humans		
		TWA	1,000 ppm 1,900 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	1,000 ppm 1,900 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		

		TWA	1,000.000000 ppm 1,900.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	1,000.000000 ppm 1,900.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		STEL	1,000.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Confirmed animal carcinogen with unknown relevance to humans		

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 30 min
Material tested:Vitoject® (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless
b)	Odour	No data available

c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -116 °C (-177 °F)
f)	Initial boiling point and boiling range	34.6 °C (94.3 °F) at 1,013 hPa (760 mmHg)
g)	Flash point	-40 °C (-40 °F) - closed cup - DIN 51755 Part 1
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 48 %(V) Lower explosion limit: 1.8 %(V)
k)	Vapour pressure	189 hPa (142 mmHg) at 0 °C (32 °F) 389 hPa (292 mmHg) at 10 °C (50 °F) 563 hPa (422 mmHg) at 20 °C (68 °F) 863 hPa (647 mmHg) at 30 °C (86 °F) 1,228 hPa (921 mmHg) at 40 °C (104 °F) 2,311 hPa (1,733 mmHg) at 60 °C (140 °F)
l)	Vapour density	2.56 - (Air = 1.0)
m)	Relative density	0.71 g/cm3 at 20 °C (68 °F)
n)	Water solubility	65 g/l at 20 °C (68 °F)
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density	2.56 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.
Contains the following stabiliser(s):
Ethanol (2 %)
BHT (10 ppm)

10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials
Oxidizing agents, Strong acids

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 1,215 mg/kg
(OECD Test Guideline 401)

LDLo Oral - Human - 260 mg/kg
Remarks: (RTECS)

LD50 Oral - Rat - 1,215 mg/kg
Remarks: (RTECS)

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Dermatitis

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitisation
Sensitisation test: - Mouse
Result: negative
(OECD Test Guideline 429)

Human experience
Result: negative
Remarks: (Lit.)

Germ cell mutagenicity
No data available

Mutagenicity (mammal cell test): chromosome aberration.
Human lymphocytes
Result: negative

Mutagenicity (mammal cell test):
Mouse lymphoma test
Result: negative

Ames test
Salmonella typhimurium
Result: negative
(IUCLID)

OECD Test Guideline 474
Mouse
Result: negative

Carcinogenicity

No data available

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
May cause drowsiness or dizziness. - Central nervous system
Acute oral toxicity - Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: KI5775000

Inhalation may provoke the following symptoms:
Cough, chest pain, Difficulty in breathing, Dizziness, Drowsiness, Contact with eyes can cause:, Redness, Provokes tears., Blurred vision, Prolonged or repeated exposure to skin causes defatting and dermatitis.

Liver - Ingestion may provoke the following symptoms:, Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence
Liver - Ingestion may provoke the following symptoms:, Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence (Ethanol)

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 2,840 mg/l - 48 h Remarks: (ECOTOX Database)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 1,380 mg/l - 48 h Remarks: (IUCLID)
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 21,000 mg/l - 3 h (OECD Test Guideline 209)
	static test NOEC - activated sludge - 42 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability
Biodegradability Result: - Not readily biodegradable.

12.3 Bioaccumulative potential
No bioaccumulation is to be expected (log Pow <= 4).

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1155 Class: 3 Packing group: I
Proper shipping name: Diethyl ether
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 1155 Class: 3 Packing group: I EMS-No: F-E, S-D
Proper shipping name: DIETHYL ETHER

IATA
UN number: 1155 Class: 3 Packing group: I
Proper shipping name: Diethyl ether

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Diethyl ether	60-29-7	1993-04-24
Ethanol	64-17-5	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Diethyl ether	60-29-7	1993-04-24
Ethanol	64-17-5	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Diethyl ether	60-29-7	1993-04-24
Ethanol	64-17-5	2007-03-01

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H224	Extremely flammable liquid and vapour.
H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
STOT SE	Specific target organ toxicity - single exposure

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	4
Physical Hazard	2

NFPA Rating

Health hazard:	2
Fire Hazard:	4
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.7 Revision Date: 02/02/2018 Print Date: 11/10/2018

Silver Nitrate

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 11/21/1998 Revision date: 02/20/2018 Supersedes: 02/20/2018 Version: 1.1

SECTION 1: Identification

1.1. Identification

Product form	:	Substance
Substance name	:	Silver Nitrate
CAS-No.	:	7761-88-8
Product code	:	LC22500
Formula	:	AgNO3
Synonyms	:	argent nitrate / azote d'argent / lunar caustic / nitrate of silver / nitric acid silver salt / nitric acid silver(1+) salt / pierre infernale / salpetersaures Silber / Silbersalpeter / silver mononitrate / silver nitrate / silver(I) nitrate / silver(I) salt nitric acid

1.2. Recommended use and restrictions on use

Use of the substance/mixture	:	Laboratory chemical Chemical intermediate Water treatment Oxidant Photographic chemical: component Cosmetic product: dyestuff
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
info@labchem.com - www.labchem.com

1.4. Emergency telephone number

Emergency number : CHEMTREC: 1-800-424-9300 or 011-703-527-3887

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Oxidizing solids Category 2	H272	May intensify fire; oxidizer
Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Skin corrosion/irritation Category 1B	H314	Causes severe skin burns and eye damage
Serious eye damage/eye irritation Category 1	H318	Causes serious eye damage
Hazardous to the aquatic environment - Acute Hazard Category 1	H400	Very toxic to aquatic life
Hazardous to the aquatic environment - Chronic Hazard Category 1	H410	Very toxic to aquatic life with long lasting effects

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS03 GHS05 GHS07 GHS09

Signal word (GHS-US) : Danger

Hazard statements (GHS-US) : H272 - May intensify fire; oxidizer
H302 - Harmful if swallowed

H314 - Causes severe skin burns and eye damage
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US) : P210 - Keep away from heat, open flames, sparks. - No smoking.
P220 - Keep/Store away from combustible materials
P221 - Take any precaution to avoid mixing with combustibles
P260 - Do not breathe dust.
P264 - Wash exposed skin thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P273 - Avoid release to the environment.
P280 - Wear eye protection, face protection, protective gloves, protective clothing.
P301+P330+P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303+P361+P353 - IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304+P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position 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
P310 - Immediately call a poison center or doctor/physician.
P363 - Wash contaminated clothing before reuse.
P391 - Collect spillage.
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 : Mono-constituent

Name	Product identifier	%	GHS-US classification
Silver Nitrate (Main constituent)	(CAS-No.) 7761-88-8	100	Ox. Sol. 2, H272 Acute Tox. 4 (Oral), H302 Skin Corr. 1B, H314 Eye Dam. 1, H318 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

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.

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 (15 minutes)/shower. Do not apply (chemical) neutralizing agents. Remove clothing while washing. Do not remove clothing if it sticks to the skin. Cover wounds with sterile bandage. If burned surface > 10%: take victim to hospital.

First-aid measures after eye contact : Rinse immediately with plenty of water for 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Do not apply neutralizing agents. Take victim to an ophthalmologist.

First-aid measures after ingestion : Rinse mouth with water. Immediately after ingestion: give lots of water to drink. Do not induce vomiting. Immediately consult a doctor/medical service. Doctor: administration of chemical antidote. Call Poison Information Centre (www.big.be/antigif.htm). Ingestion of large quantities: immediately to hospital.

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

Symptoms/effects : Not expected to present a significant hazard under anticipated conditions of normal use.

Symptoms/effects after inhalation	:	AFTER INHALATION OF DUST: Dry/sore throat. Coughing. FOLLOWING SYMPTOMS MAY APPEAR LATER: Risk of lung edema.
Symptoms/effects after skin contact	:	Caustic burns/corrosion of the skin.
Symptoms/effects after eye contact	:	Corrosion of the eye tissue. Permanent eye damage.
Symptoms/effects after ingestion	:	AFTER ABSORPTION OF LARGE QUANTITIES: Burns to the gastric/intestinal mucosa. Vomiting. Abdominal pain. Diarrhoea. Shock. Dizziness. Low arterial pressure. Disturbances of consciousness. Cramps/uncontrolled muscular contractions. Respiratory collapse.
Chronic symptoms	:	ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: May stain the skin. Blue/grey discoloration of the skin. Inflammation/damage of the eye tissue. Visual disturbances. Possible inflammation of the respiratory tract.

4.3. Immediate medical attention and special treatment, if necessary

Obtain medical assistance. Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	:	Adapt extinguishing media to the environment for surrounding fires.

5.2. Specific hazards arising from the chemical

Fire hazard	:	DIRECT FIRE HAZARD. Non combustible. INDIRECT FIRE HAZARD. May intensify fire; oxidiser. Reactions involving a fire hazard: see "Reactivity Hazard".
Explosion hazard	:	INDIRECT EXPLOSION HAZARD. Reactions with explosion hazards: see "Reactivity Hazard".
Reactivity	:	Decomposes on exposure to light. This reaction is accelerated on exposure to impurities. Violent to explosive reaction with many compounds e.g.: with (strong) reducers. Violent to explosive reaction with combustible materials: risk of spontaneous ignition.

5.3. Special protective equipment and precautions for fire-fighters

Precautionary measures fire	:	Exposure to fire/heat: keep upwind. Exposure to fire/heat: consider evacuation. Exposure to fire/heat: have neighbourhood close doors and windows.
Firefighting instructions	:	Cool tanks/drums with water spray/remove them into safety. Cool from behind cover/unmanned monitors. Dilute toxic gases with water spray. Take account of toxic fire-fighting water. Use water moderately and if possible collect or contain it.
Protection during firefighting	:	Heat/fire exposure: compressed air/oxygen apparatus.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Protective equipment	:	Gloves. Face-shield. Corrosion-proof suit. Dust cloud production: compressed air/oxygen apparatus.
Emergency procedures	:	Mark the danger area. Prevent dust cloud formation. No naked flames. Keep containers closed. Wash contaminated clothes. In case of hazardous reactions: keep upwind. In case of reactivity hazard: consider evacuation.
Measures in case of dust release	:	In case of dust production: keep upwind. In case of dust production: consider evacuation. Dust production: have neighbourhood close doors and windows.

6.1.2. For emergency responders

Protective equipment	:	Equip cleanup crew with proper protection.
Emergency procedures	:	Ventilate area. Stop release.

6.2. Environmental precautions

Prevent soil and water pollution. Prevent spreading in sewers.

6.3. Methods and material for containment and cleaning up

For containment	:	Contain released substance, pump into suitable containers. Plug the leak, cut off the supply. Dam up the solid spill. Knock down/dilute dust cloud with water spray. Take account of toxic/corrosive precipitation water.
Methods for cleaning up	:	Prevent dispersion by covering with dry sand. Scoop solid spill into closing containers or synthetic bags. Carefully collect the spill/leftovers. Spill must not return in its original container. 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

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	:	Avoid raising dust. Keep away from naked flames/heat. Measure the concentration in the air regularly. Carry operations in the open/under local exhaust/ventilation or with respiratory protection. Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Keep the substance free from contamination. Thoroughly clean/dry the installation before use. Do not discharge the waste into the drain.
Hygiene measures	:	Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions	:	Keep only in the original container in a cool, well ventilated place away from : combustible materials, incompatible materials. Keep container closed when not in use.
Incompatible products	:	Strong bases. combustible materials. Sodium hypochlorite. Strong acids.
Incompatible materials	:	Combustible material. Sources of ignition. Direct sunlight.
Heat-ignition	:	KEEP SUBSTANCE AWAY FROM: heat sources.
Prohibitions on mixed storage	:	KEEP SUBSTANCE AWAY FROM: combustible materials. reducing agents. (strong) bases. organic materials. alcohols.
Storage area	:	Store in a cool area. Store in a dry area. Store in a dark area. Keep container in a well-ventilated place. Keep locked up. Unauthorized persons are not admitted. Meet the legal requirements. Keep only in the original container.
Special rules on packaging	:	SPECIAL REQUIREMENTS: closing. watertight. clean. opaque. correctly labelled. meet the legal requirements. Secure fragile packagings in solid containers.
Packaging materials	:	SUITABLE MATERIAL: iron. synthetic material.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Silver Nitrate (7761-88-8)		
ACGIH	ACGIH TWA (mg/m³)	0.01 mg/m³
OSHA	OSHA PEL (TWA) (mg/m³)	0.01 mg/m³
IDLH	US IDLH (mg/m³)	10 mg/m³
NIOSH	NIOSH REL (TWA) (mg/m³)	0.01 mg/m³

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:

Gloves. Safety glasses. Chemical resistant apron. Face shield. Protective clothing. Dust production: dust mask with filter type P3.

Materials for protective clothing:

GIVE GOOD RESISTANCE: butyl rubber. neoprene. PVA

Hand protection:

Gloves

Eye protection:

Face shield. In case of dust production: protective goggles

Skin and body protection:

Corrosion-proof clothing. In case of dust production: head/neck protection

Respiratory protection:

Dust production: dust mask with filter type P3.
High dust production: self-contained breathing apparatus

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Solid
Appearance	:	Crystalline solid.
Color	:	Colourless to grey On exposure to light: dark grey to black
Odor	:	Odorless
Odor threshold	:	No data available
pH	:	7
Melting point	:	212 °C
Freezing point	:	No data available
Boiling point	:	444 °C
Flash point	:	Not applicable
Relative evaporation rate (butyl acetate=1)	:	No data available
Flammability (solid, gas)	:	Non flammable.
Vapor pressure	:	< 0.1 hPa (20 °C)
Relative vapor density at 20 °C	:	5.8
Relative density	:	4.3
Specific gravity / density	:	4352 kg/m³
Molecular mass	:	169.87 g/mol
Solubility	:	Soluble in water. Substance sinks in water. Soluble in ammonia. Soluble in glycerol. Water: 144 g/100ml Acetone: 0.4 g/100ml
Log Pow	:	0.19 (Estimated value)
Auto-ignition temperature	:	No data available
Decomposition temperature	:	444 °C
Viscosity, kinematic	:	No data available
Viscosity, dynamic	:	No data available
Explosion limits	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	May intensify fire; oxidiser.

9.2. Other information

VOC content	:	0 %
Other properties	:	Translucent. Substance has neutral reaction.

SECTION 10: Stability and reactivity

10.1. Reactivity

Decomposes on exposure to light. This reaction is accelerated on exposure to impurities. Violent to explosive reaction with many compounds e.g.: with (strong) reducers. Violent to explosive reaction with combustible materials: risk of spontaneous ignition.

10.2. Chemical stability

Unstable on exposure to light.

10.3. Possibility of hazardous reactions

Not established.

10.4. Conditions to avoid

Direct sunlight. High temperature. Extremely high or low temperatures.

10.5. Incompatible materials

combustible materials. Strong bases. Strong reducing agents. Strong acids.

10.6. Hazardous decomposition products

Nitrogen oxides. fume. Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure : Inhalation; Skin and eye contact

Acute toxicity : Oral: Harmful if swallowed.

Silver Nitrate (7761-88-8)	
LD50 oral rat	1173 mg/kg (Rat)
ATE US (oral)	1173 mg/kg body weight

Skin corrosion/irritation : Causes severe skin burns and eye damage.
pH: 7

Serious eye damage/irritation : Causes serious eye damage.
pH: 7

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

Specific target organ toxicity – single exposure : Not classified

Specific target organ toxicity – repeated exposure : Not classified

Aspiration hazard : Not classified

Potential Adverse human health effects and symptoms : Based on available data, the classification criteria are not met.

Symptoms/effects after inhalation : AFTER INHALATION OF DUST: Dry/sore throat. Coughing. FOLLOWING SYMPTOMS MAY APPEAR LATER: Risk of lung edema.

Symptoms/effects after skin contact : Caustic burns/corrosion of the skin.

Symptoms/effects after eye contact : Corrosion of the eye tissue. Permanent eye damage.

Symptoms/effects after ingestion : AFTER ABSORPTION OF LARGE QUANTITIES: Burns to the gastric/intestinal mucosa. Vomiting. Abdominal pain. Diarrhoea. Shock. Dizziness. Low arterial pressure. Disturbances of consciousness. Cramps/uncontrolled muscular contractions. Respiratory collapse.

Chronic symptoms : ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: May stain the skin. Blue/grey discoloration of the skin. Inflammation/damage of the eye tissue. Visual disturbances. Possible inflammation of the respiratory tract.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Dangerous for the environment.

Ecology - air : Not classified as dangerous for the ozone layer (Regulation (EC) No 1005/2009).

Ecology - water : Very toxic to crustacea. Very toxic to fishes. Severe water pollutant (surface water). Very toxic to algae. May cause eutrophication.

Silver Nitrate (7761-88-8)	
LC50 fish 1	0.006 mg/l (96 h, Salmo gairdneri, Flow-through system)
EC50 Daphnia 1	0.0006 mg/l (48 h, Daphnia magna)

12.2. Persistence and degradability

Silver Nitrate (7761-88-8)	
Persistence and degradability	Biodegradability: not applicable.
Biochemical oxygen demand (BOD)	Not applicable
Chemical oxygen demand (COD)	Not applicable

Silver Nitrate (7761-88-8)	
ThOD	Not applicable
BOD (% of ThOD)	Not applicable

12.3. Bioaccumulative potential

Silver Nitrate (7761-88-8)	
BCF fish 1	11 - 19 (Micropterus salmoides, Chronic)
BCF fish 2	15 - 150 (Lepomis macrochirus, Chronic)
Log Pow	0.19 (Estimated value)
Bioaccumulative potential	Low potential for bioaccumulation (BCF < 500).

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Other information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Disposal methods

Regional legislation (waste) : Disposal must be done according to official regulations.

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

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/reuse. Remove to an authorized dump (Class I).

Additional information : Hazardous waste according to Directive 2008/98/EC, as amended by Regulation (EU) No 1357/2014 and Regulation (EU) No 2017/997.

Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN1493 Silver nitrate, 5.1, II

UN-No.(DOT) : UN1493

Proper Shipping Name (DOT) : Silver nitrate

Packing group (DOT) : II - Medium Danger

Hazard labels (DOT) : 5.1 - Oxidizer

Dangerous for the environment : Yes

Marine pollutant : Yes

DOT Packaging Non Bulk (49 CFR 173.xxx) : 212

DOT Packaging Bulk (49 CFR 173.xxx) : 242

DOT Special Provisions (49 CFR 172.102)	:	IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2). IP2 - When IBCs other than metal or rigid plastics IBCs are used, they must be offered for transportation in a closed freight container or a closed transport vehicle. IP4 - Flexible, fiberboard or wooden IBCs must be sift-proof and water-resistant or be fitted with a sift-proof and water-resistant liner. T3 - 2.65 178.274(d)(2) Normal..... 178.275(d)(2) TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
DOT Packaging Exceptions (49 CFR 173.xxx)	:	152
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	:	5 kg
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	:	25 kg
DOT Vessel Stowage Location	:	A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
Other information	:	No supplementary information available.

SECTION 15: Regulatory information

15.1. US Federal regulations

Silver Nitrate (7761-88-8)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory	
RQ (Reportable quantity, section 304 of EPA's List of Lists)	1 lb

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

15.2. International regulations

CANADA

Silver Nitrate (7761-88-8)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

Silver Nitrate (7761-88-8)
Listed on the Canadian IDL (Ingredient Disclosure List)

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

Revision date	:	02/20/2018
Other information	:	None.

Full text of H-phrases: see section 16:

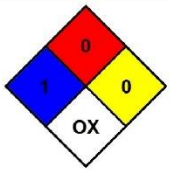
H272	May intensify fire; oxidizer
H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

NFPA health hazard : 1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA fire hazard : 0 - Materials that will not burn under typical dire 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.

NFPA specific hazard : OX - Materials that posses oxidizing properties.



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 : F

F - Safety glasses, Gloves, Synthetic apron, Dust respirator

SDS US LabChem

Information in this SDS is from available published sources and is believed to be accurate. No warranty, express or implied, is made and LabChem Inc assumes no liability resulting from the use of this SDS. The user must determine suitability of this information for his application.

SAFETY DATA SHEET

Version 6.4
Revision Date 10/02/2017
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Methanol

Product Number : 322415
Brand : Sigma-Aldrich
Index-No. : 603-001-00-X

CAS-No. : 67-56-1

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), H370

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)
H225 Highly flammable liquid and vapour.
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled.
H370 Causes damage to organs.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use only non-sparking tools.

P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash 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 protective gloves/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Methyl alcohol
Formula	:	CH_4O
Molecular weight	:	32.04 g/mol
CAS-No.	:	67-56-1
EC-No.	:	200-659-6
Index-No.	:	603-001-00-X
Registration number	:	01-2119433307-44-XXXX

Hazardous components

Component	Classification	Concentration
Methanol		
	Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301 + H311 + H331, H370	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		STEL	250.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		TWA	200.000000 ppm 260.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		ST	250.000000 ppm 325.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200.000000 ppm 260.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Headache Nausea Dizziness Eye damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption		
		TWA	200 ppm 260 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		

		ST	250 ppm 325 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		STEL	250 ppm 325 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	200 ppm 260 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methanol	67-56-1	Methanol	15.0000 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			
		Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

Derived No Effect Level (DNEL)

Application Area	Exposure routes	Health effect	Value
Workers	Skin contact	Long-term systemic effects	40mg/kg BW/d
Consumers	Skin contact	Long-term systemic effects	8mg/kg BW/d
Consumers	Ingestion	Long-term systemic effects	8mg/kg BW/d
Workers	Skin contact	Acute systemic effects	40mg/kg BW/d
Consumers	Skin contact	Acute systemic effects	8mg/kg BW/d
Consumers	Ingestion	Acute systemic effects	8mg/kg BW/d
Workers	Inhalation	Acute systemic effects	260 mg/m3
Workers	Inhalation	Acute local effects	260 mg/m3
Workers	Inhalation	Long-term systemic effects	260 mg/m3
Workers	Inhalation	Long-term local effects	260 mg/m3
Consumers	Inhalation	Acute systemic effects	50 mg/m3
Consumers	Inhalation	Acute local effects	50 mg/m3
Consumers	Inhalation	Long-term systemic effects	50 mg/m3
Consumers	Inhalation	Long-term local effects	50 mg/m3

Predicted No Effect Concentration (PNEC)

Compartment	Value
Soil	23.5 mg/kg

Marine water	15.4 mg/l
Fresh water	154 mg/l
Fresh water sediment	570.4 mg/kg
Onsite sewage treatment plant	100 mg/kg

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 31 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless
b)	Odour	pungent
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -98 °C (-144 °F)

f)	Initial boiling point and boiling range	64.7 °C (148.5 °F)
g)	Flash point	9.7 °C (49.5 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 36 %(V) Lower explosion limit: 6 %(V)
k)	Vapour pressure	130.3 hPa (97.7 mmHg) at 20.0 °C (68.0 °F) 546.6 hPa (410.0 mmHg) at 50.0 °C (122.0 °F) 169.27 hPa (126.96 mmHg) at 25.0 °C (77.0 °F)
l)	Vapour density	1.11
m)	Relative density	0.791 g/mL at 25 °C (77 °F)
n)	Water solubility	completely miscible
o)	Partition coefficient: n-octanol/water	log Pow: -0.77
p)	Auto-ignition temperature	455.0 °C (851.0 °F) at 1,013 hPa (760 mmHg)
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	Not explosive
t)	Oxidizing properties	The substance or mixture is not classified as oxidizing.

9.2 Other safety information

Minimum ignition energy	0.14 mJ
Conductivity	< 1 µS/cm
Relative vapour density	1.11

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
Acid chlorides, Acid anhydrides, Oxidizing agents, Alkali metals, Reducing agents, Acids

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LDLO Oral - Human - 143 mg/kg
Remarks: Lungs, Thorax, or Respiration:Dyspnea. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhoea.

LD50 Oral - Rat - 1,187 - 2,769 mg/kg

LC50 Inhalation - Rat - 4 h - 128.2 mg/l

LC50 Inhalation - Rat - 6 h - 87.6 mg/l

LD50 Dermal - Rabbit - 17,100 mg/kg

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation

Respiratory or skin sensitisation
Maximisation Test - Guinea pig
Does not cause skin sensitisation.
(OECD Test Guideline 406)

Germ cell mutagenicity
Ames test
S. typhimurium
Result: negative

in vitro assay
fibroblast
Result: negative
Mutation in mammalian somatic cells.

Mutagenicity (in vivo mammalian bone-marrow cytogenetic test, chromosomal analysis)
Mouse - male and female
Result: negative

Carcinogenicity

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
Damage to fetus not classifiable

Fertility classification not possible from current data.

Specific target organ toxicity - single exposure
Causes damage to organs.

Specific target organ toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
No aspiration toxicity classification

Additional Information
RTECS: PC1400000

Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures., Methyl alcohol may be fatal or cause blindness if swallowed.
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	mortality LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h
	NOEC - Oryzias latipes - 7,900 mg/l - 200 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - > 10,000.00 mg/l - 48 h
Toxicity to algae	Growth inhibition EC50 - Scenedesmus capricornutum (fresh water algae) - 22,000.0 mg/l - 96 h

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 5 d Result: 72 % - rapidly biodegradable
Biochemical Oxygen Demand (BOD)	600 - 1,120 mg/g
Chemical Oxygen Demand (COD)	1,420 mg/g
Theoretical oxygen demand	1,500 mg/g

12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 72 d at 20 °C - 5 mg/l Bioconcentration factor (BCF): 1.0

12.4 Mobility in soil
Will not adsorb on soil.

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

Additional ecological information	Avoid release to the environment.
Stability in water	at 19 °C83 - 91 % - 72 h Remarks: Hydrolyses on contact with water.Hydrolyses readily.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1230 Class: 3 Packing group: II
Proper shipping name: Methanol
Reportable Quantity (RQ): 5000 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOL

IATA
UN number: 1230 Class: 3 (6.1) Packing group: II
Proper shipping name: Methanol

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

California Prop. 65 Components

	CAS-No.	Revision Date
WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm. Methanol	67-56-1	2012-03-16

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H370	Causes damage to organs.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	3
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 6.4 Revision Date: 10/02/2017 Print Date: 11/10/2018

SAFETY DATA SHEET

Version 5.10
Revision Date 09/10/2018
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Sodium hydroxide solution

Product Number : 415413
Brand : Sigma-Aldrich

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Corrosive to metals (Category 1), H290
Skin corrosion (Category 1A), H314
Serious eye damage (Category 1), H318
Acute aquatic toxicity (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H402	Harmful to aquatic life.

Precautionary statement(s)

P234	Keep only in original container.
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P363	Wash contaminated clothing before reuse.
P390	Absorb spillage to prevent material damage.
P405	Store locked up.
P406	Store in corrosive resistant container with a resistant inner liner.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures

Formula : HNaO
Molecular weight : 40.00 g/mol

Hazardous components

Component		Classification	Concentration
Sodium hydroxide			
CAS-No.	1310-73-2	Met. Corr. 1; Skin Corr. 1A; Eye Dam. 1; Aquatic Acute 3; H290, H314, H402	50 - 70 %
EC-No.	215-185-5		
Index-No.	011-002-00-6		
Registration number	01-2119457892-27-XXXX		

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.Continue rinsing eyes during transport to hospital.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid inhalation of vapour or mist.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): 8B: Non-combustible, corrosive hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Sodium hydroxide	1310-73-2	C	2 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Eye irritation Skin irritation		
		C	2 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	2 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	2 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	14.0
e)	Melting point/freezing point	-12 - 10 °C (10 - 50 °F)
f)	Initial boiling point and boiling range	105 - 140 °C (221 - 284 °F)
g)	Flash point	Not applicable
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or	No data available

	explosive limits	
k)	Vapour pressure	< 24 hPa (< 18 mmHg) at 20 °C (68 °F)
l)	Vapour density	1.38 - (Air = 1.0)
m)	Relative density	1.515 g/mL at 25 °C (77 °F)
n)	Water solubility	completely miscible, soluble
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density	1.38 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Water, acids, Organic materials, Chlorinated solvents, Aluminum, Phosphorus, Tin/tin oxides, Zinc

10.6 Hazardous decomposition products
Other decomposition products - No data available
Hazardous decomposition products formed under fire conditions. - Sodium oxides
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
No data available

Inhalation: No data available

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: Not available

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1824 Class: 8 Packing group: II
Proper shipping name: Sodium hydroxide solution

Reportable Quantity (RQ): 2000 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 1824 Class: 8 Packing group: II EMS-No: F-A, S-B
Proper shipping name: SODIUM HYDROXIDE SOLUTION

IATA
UN number: 1824 Class: 8 Packing group: II
Proper shipping name: Sodium hydroxide solution

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Sodium hydroxide	1310-73-2	1989-08-11

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Water	7732-18-5	
Sodium hydroxide	1310-73-2	1989-08-11

New Jersey Right To Know Components

	CAS-No.	Revision Date
Water	7732-18-5	
Sodium hydroxide	1310-73-2	1989-08-11

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Eye Dam.	Serious eye damage
H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H402	Harmful to aquatic life.
Met. Corr.	Corrosive to metals
Skin Corr.	Skin corrosion

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.10 Revision Date: 09/10/2018 Print Date: 11/10/2018

SAFETY DATA SHEET
according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 01/16/2018 Version 2.1

SECTION 1.Identification

Product identifier

Product number	101514
Product name	Hydrochloric acid 30% Ultrapur

Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Reagent for analysis, Chemical production

Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) MilliporeSigma is a business of Merck KGaA, Darmstadt, Germany.
Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. Hazards Identification

GHS Classification

Corrosive to Metals, Category 1, H290
Skin corrosion, Category 1B, H314
Serious eye damage, Category 1, H318
Specific target organ systemic toxicity - single exposure, Category 3, Respiratory system, H335
For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms

Signal Word
Danger

Hazard Statements
H290 May be corrosive to metals.
H314 Causes severe skin burns and eye damage.
H335 May cause respiratory irritation.

Precautionary Statements

P234 Keep only in original container.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P310 Immediately call a POISON CENTER/doctor.
P321 Specific treatment (see supplemental first aid instructions on this label).
P363 Wash contaminated clothing before reuse.
P390 Absorb spillage to prevent material damage.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P406 Store in corrosive resistant stainless steel container with a resistant inner liner.
P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Chemical nature Aqueous solution

Hazardous ingredients

Chemical name (Concentration)
CAS-No.
hydrochloric acid (>= 30 % - < 50 %)

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

General advice
First aider needs to protect himself.

Inhalation
After inhalation: fresh air. Call in physician.

Skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

Eye contact
After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

Ingestion
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation!). Call a physician immediately. Do not attempt to neutralize.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed
Irritation and corrosion, Cough, Shortness of breath, cardiovascular disorders, Risk of blindness!

Indication of any immediate medical attention and special treatment needed
No information available.

SECTION 5. Fire-fighting measures

Extinguishing media
Suitable extinguishing media
Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture
Not combustible.
Ambient fire may liberate hazardous vapors.
Fire may cause evolution of:
Hydrogen chloride gas

Advice for firefighters
Special protective equipment for fire-fighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions
Do not let product enter drains.

Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up with liquid-absorbent and neutralizing material (e.g. Chemizorb® H^+, Art. No. 101595).
Dispose of properly. Clean up affected area.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Requirements for storage areas and containers

No metal containers.

Tightly closed.

Store at +5°C to +30°C (+41°F to +86°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
hydrochloric acid			
ACGIH	Ceiling Limit Value:	2 ppm	
NIOSH/GUIDE	Ceiling Limit Value and Time Period (if specified):	5 ppm 7 mg/m³	
OSHA_TRANS	Ceiling Limit Value:	5 ppm 7 mg/m³	
Z1A	Ceiling Limit Value:	5 ppm 7 mg/m³	

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0.11 mm
Break through time:	> 480 min

splash contact:

Glove material:	natural latex

Glove thickness:	0.6 mm
Break through time:	> 120 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 706 Lapren® (splash contact).
The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.
This recommendation applies only to the product stated in the safety data sheet and supplied by us as well as to the purpose specified by us. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment:
Acid-resistant protective clothing.

Respiratory protection
required when vapors/aerosols are generated.
Recommended Filter type: filter E-(P2)
The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are performed according to the instructions of the producer. These measures have to be properly documented.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	light yellow
Odor	stinging
Odor Threshold	No information available.
pH	< 1 at 300 g/l 68 °F (20 °C)
Melting point	-58 °F (-50 °C)
Boiling point/boiling range	185 °F (85 °C) at 1,013 hPa
Flash point	Not applicable
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	Not applicable
Upper explosion limit	Not applicable

Vapor pressure	21.8 hPa at 68 °F (20 °C)
Relative vapor density	No information available.
Density	1.15 g/cm3 at 68 °F (20 °C)
Relative density	No information available.
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	Not applicable
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	1.74 mPa.s
Explosive properties	Not classified as explosive.
Oxidizing properties	none
Ignition temperature	Not applicable
Corrosion	May be corrosive to metals.

SECTION 10. Stability and reactivity

Reactivity

Corrosive in contact with metals

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Exothermic reaction with:

Amines, potassium permanganate, salts of oxyhalogenic acids, semimetallic oxides, semimetallic hydrogen compounds, Aldehydes, vinylmethyl ether

Risk of ignition or formation of inflammable gases or vapors with:

carbides, lithium silicide, Fluorine

Generates dangerous gases or fumes in contact with:

Aluminum, hydrides, formaldehyde, Metals, strong alkalis, Sulfides

Risk of explosion with:

Alkali metals, conc. sulfuric acid

Conditions to avoid
Heating.

Incompatible materials
Metals, metal alloys
Gives off hydrogen by reaction with metals.

Hazardous decomposition products
in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Inhalation, Eye contact, Skin contact

Target Organs
Eyes
Skin
Respiratory system
Cornea

Acute oral toxicity
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Skin irritation

Mixture causes burns.

Eye irritation
Mixture causes serious eye damage. Risk of blindness!

Specific target organ systemic toxicity - single exposure
May cause respiratory irritation.
Target Organs: Respiratory system

Specific target organ systemic toxicity - repeated exposure
The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No component of this product present at levels greater than or

	equal to 0.1% is on OSHA’ s list of regulated carcinogens.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

After uptake:
After a latency period:
cardiovascular disorders
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

Ingredients

hydrochloric acid

Skin irritation
Rabbit
Result: Corrosive
OECD Test Guideline 404

Eye irritation
Rabbit
Result: Irreversible effects on the eye
OECD Test Guideline 405

Sensitization
Maximization Test Guinea pig
Result: Does not cause skin sensitization.
Method: OECD Test Guideline 406

SECTION 12. Ecological information

Ecotoxicity

No information available.

Persistence and degradability

No information available.

Bioaccumulative potential

Partition coefficient: n-octanol/water
Not applicable

Mobility in soil

No information available.

Additional ecological information
Forms corrosive mixtures with water even if diluted. Harmful effect due to pH shift.
Discharge into the environment must be avoided.

Ingredients

hydrochloric acid

Toxicity to fish
Lepomis macrochirus (Bluegill sunfish): 20.5 mg/l; 96 h
OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates
EC50: 1.3 mg/l; 48 h
OECD Test Guideline 202

Substance does not meets the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 1789
Proper shipping name	HYDROCHLORIC ACID
Class	8
Packing group	II
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 1789
Proper shipping name	HYDROCHLORIC ACID
Class	8
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 1789
Proper shipping name	HYDROCHLORIC ACID
Class	8
Packing group	II
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-B

SECTION 15. Regulatory information

United States of America

SARA 313

The following components are subject to reporting levels established by SARA Title III, Section 313:

Ingredients

hydrochloric acid *30 %*

SARA 302

The following components are subject to reporting levels established by SARA Title III, Section 302:

Ingredients

hydrochloric acid

Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

Ingredients

hydrochloric acid

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

Ingredients

hydrochloric acid

DEA List I

Not listed

DEA List II

Listed

Ingredients

hydrochloric acid

US State Regulations

Massachusetts Right To Know

Ingredients

hydrochloric acid

Pennsylvania Right To Know

Ingredients

hydrochloric acid

New Jersey Right To Know

Ingredients

hydrochloric acid

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA:	All components of the product are listed in the TSCA-inventory.
DSL:	All components of this product are on the Canadian DSL

SECTION 16. Other information

Training advice
Provide adequate information, instruction and training for operators.

Labeling
Hazard pictograms

Signal Word
Danger

Hazard Statements
H290 May be corrosive to metals.
H314 Causes severe skin burns and eye damage.
H335 May cause respiratory irritation.

Precautionary Statements
Prevention
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
Response
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
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 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Full text of H-Statements referred to under sections 2 and 3.

H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.

Key or legend to abbreviations and acronyms used in the safety data sheet
Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Revision Date01/16/2018

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

25.4 Aspen Flowsheets and Summary Reports

25.4.1 Aspen Flowsheet and Summary Report for Part 1 of Process

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ASPEN TECHNOLOGY, INC.         U.S.A. 888/996-7100
781/221-6400              EUROPE (44) 1189-226555

PLATFORM: WINDOWS                    APRIL 13, 2019
VERSION: 36.0  Build 250 Patchlevel 1         SATURDAY
INSTALLATION:                       11:59:16 A.M.

ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE  I



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   BEDFORD, MA 01730.
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```

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RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: EDIT

INPUT FILE NAME: _0952vyn.inm

INPUT PROBLEM DATA FILE NAME : _0952vyn
OUTPUT PROBLEM DATA FILE NAME: _5912bjf
LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:
NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME: apmain
LOCATED IN: C:\Program Files (x86)\AspenTech\Aspen Plus V10.0\Engine\\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
MEOH-1	----	S1	GLY-1	----	S1
FAME-1	----	S1	1	S1	----
2	S1	DECANT	GLY-2	DECANT	GLYSEP
FAME-2	DECANT	FAMES	METH2	FAMES	----
CLEANFA	FAMES	B1	TOLLE	B2	B3
PROD	B2	----	METHTOP	GLYSEP	----
PUREGLY	GLYSEP	----	S1	B3	----
S3	B3	----	S2	----	B3
S4	B1	B2			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
S1	FAME-1 GLY-1 MEOH-1	1 2
DECANT	2	GLY-2 FAME-2
FAMES	FAME-2	METH2 CLEANFA
B2	S4	TOLLE PROD
GLYSEP	GLY-2	METHTOP PUREGLY
B3	TOLLE S2	S1 S3
B1	CLEANFA	S4

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
HPSTEAM REFRIG S1 DECANT GLYSEP FAMES B1 B2 B3

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

           *** MASS AND ENERGY BALANCE ***
                    IN       OUT    RELATIVE DIFF.
  CONVENTIONAL COMPONENTS (KMOL/HR )
    C14:0-ME         17.2371     17.2371    -0.346590E-06
    C16:0-ME         75.6548     75.6548    -0.346590E-06
    C16:1-ME         40.6420     40.6421    -0.346590E-06
    C18:0-ME         5.00182     5.00183    -0.346590E-06
    C18:1-ME         34.7227     34.7227    -0.346590E-06
    C18:2-ME         18.4624     18.4624    -0.346590E-06
    EPA-ME          42.3882     42.3883    -0.346590E-06
    DHA-ME          2.66369     2.66369    -0.346590E-06
    METHA-01         171.440     171.440    0.314841E-06
    CARBO-01         0.00000     0.00000     0.00000
    GLYCE-01         57.1477     57.1477    0.491473E-06
    WATER           2442.37     2442.37     0.00000
  TOTAL BALANCE
    MOLE(KMOL/HR )      2907.73     2907.73    0.156392E-15
    MASS(KG/HR  )      121858.     121858.    -0.155432E-06
    ENTHALPY(CAL/SEC )   -0.613912E+08  -0.592991E+08  -0.340774E-01
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                FLOWSHEET SECTION

OVERALL FLOWSHEET BALANCE (CONTINUED)

           *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   4043.97   KG/HR
  TOTAL CO2E PRODUCTION     4043.97   KG/HR
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 4

             PHYSICAL PROPERTIES SECTION

COMPONENTS
----------

 ID    TYPE ALIAS     NAME
  C14:0-ME C   C15H30O2-N1  METHYL-MYRISTATE
  C16:0-ME C   C17H34O2-N1  METHYL-PALMITATE
  C16:1-ME C   C17H32O2-N5  METHYL-PALMITOLEATE
  C18:0-ME C   C19H38O2-N1  METHYL-STEARATE
  C18:1-ME C   C19H36O2    METHYL-OLEATE
  C18:2-ME C   C19H34O2    METHYL-LINOLEATE
  EPA-ME  C   C21H32O2-N1  C21H32O2-N1
  DHA-ME  C   C23H34O2    C23H34O2
  METHA-01 C   CH4O      METHANOL
  CARBO-01 C   CO2       CARBON-DIOXIDE
  GLYCE-01 C   C3H8O3     GLYCEROL
  WATER  C   H2O      WATER
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 5

               U-O-S BLOCK SECTION

BLOCK: B1    MODEL: PUMP
------------------------------
  INLET STREAM:     CLEANFA
  OUTLET STREAM:     S4
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

           *** MASS AND ENERGY BALANCE ***
                    IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      239.491     239.491     0.00000
    MASS(KG/HR  )      66550.4     66550.4    -0.655980E-15
    ENTHALPY(CAL/SEC )   -0.799145E+07  -0.799128E+07  -0.212647E-04
```

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

            *** INPUT DATA ***
  PRESSURE CHANGE BAR                  0.20000
  DRIVER EFFICIENCY                    1.00000

  FLASH SPECIFICATIONS:
  LIQUID PHASE CALCULATION
  NO FLASH PERFORMED
  MAXIMUM NUMBER OF ITERATIONS              30
  TOLERANCE                        0.000100000

             *** RESULTS ***
  VOLUMETRIC FLOW RATE L/MIN            1,471.63
  PRESSURE CHANGE BAR                   0.20000
  NPSH AVAILABLE  M-KGF/KG                 0.0
  FLUID POWER KW                        0.49054
  BRAKE POWER KW                        0.71149
  ELECTRICITY KW                        0.71149
  PUMP EFFICIENCY USED                     0.68946
  NET WORK REQUIRED KW                     0.71149
  HEAD DEVELOPED M-KGF/KG                  2.70589

BLOCK: B2    MODEL: FSPLIT
------------------------------
  INLET STREAM:     S4
  OUTLET STREAMS:    TOLLE    PROD
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 6

               U-O-S BLOCK SECTION

BLOCK: B2    MODEL: FSPLIT (CONTINUED)

           *** MASS AND ENERGY BALANCE ***
                   IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      239.491     239.491     0.00000
    MASS(KG/HR  )      66550.4     66550.4    -0.218660E-15
    ENTHALPY(CAL/SEC )   -0.799128E+07  -0.799128E+07   0.00000

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

            *** INPUT DATA ***

 FRACTION OF FLOW         STRM=TOLLE  FRAC=     0.11460

 STREAM CALCULATION ORDER:
    STREAM     ORDER
     TOLLE     1
     PROD      2

             *** RESULTS ***

 STREAM= TOLLE     SPLIT=     0.11460   KEY= 0  STREAM-ORDER=  1
     PROD              0.88540      0          2

BLOCK: B3    MODEL: HEATX
------------------------------
  HOT SIDE:
  ---------
  INLET STREAM:       TOLLE
```

```
  OUTLET STREAM:      S1
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:       S2
  OUTLET STREAM:      S3
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

           *** MASS AND ENERGY BALANCE ***
                  IN       OUT    RELATIVE DIFF.
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 7

               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX (CONTINUED)
  TOTAL BALANCE
    MOLE(KMOL/HR )      2469.82     2469.82     0.00000
    MASS(KG/HR  )      51626.7     51626.7     0.00000
    ENTHALPY(CAL/SEC )   -0.476515E+08  -0.476515E+08  0.156356E-15

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

             *** INPUT DATA ***

  FLASH SPECS FOR HOT SIDE:
  TWO  PHASE   FLASH
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

  FLASH SPECS FOR COLD SIDE:
  TWO  PHASE   FLASH
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

  FLOW DIRECTION AND SPECIFICATION:
   COUNTERCURRENT  HEAT EXCHANGER
   SPECIFIED COLD TEMP CHANGE
   SPECIFIED VALUE        C            16.6667
   LMTD CORRECTION FACTOR                 1.00000

  PRESSURE SPECIFICATION:
   HOT SIDE PRESSURE DROP    BAR           0.0000
   COLD SIDE PRESSURE DROP    BAR           0.0000

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
   HOT LIQUID  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT LIQUID  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT LIQUID  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD VAPOR    CAL/SEC-SQCM-K      0.0203
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 8

               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX (CONTINUED)

            *** OVERALL RESULTS ***

  STREAMS:
          ---------------------------------------
          |                     |
  TOLLE   ----->|        HOT          |-----> S1
  T= 2.3546D+02 |                     |    T= 3.4485D+01
```

```
  P= 1.2000D+00 |                   |    P= 1.2000D+00
  V= 0.0000D+00 |                   |    V= 0.0000D+00
          |                 |
  S3    <-----|        COLD       |<----- S2
  T= 4.8889D+01 |                   |    T= 3.2222D+01
  P= 1.0000D+00 |                   |    P= 1.0000D+00
  V= 0.0000D+00 |                   |    V= 0.0000D+00
         ------------------------------------

  DUTY AND AREA:
   CALCULATED HEAT DUTY      CAL/SEC       234911.1175
   CALCULATED (REQUIRED) AREA   SQM           27.7014
   ACTUAL EXCHANGER AREA     SQM           27.7014
   PER CENT OVER-DESIGN                   0.0000

  HEAT TRANSFER COEFFICIENT:
   AVERAGE COEFFICIENT (DIRTY)  CAL/SEC-SQCM-K      0.0203
   UA (DIRTY)           CAL/SEC-K       5623.9056

  LOG-MEAN TEMPERATURE DIFFERENCE:
   LMTD CORRECTION FACTOR                 1.0000
   LMTD (CORRECTED)        C             41.7701
   NUMBER OF SHELLS IN SERIES                1

  PRESSURE DROP:
   HOTSIDE, TOTAL          BAR           0.0000
   COLDSIDE, TOTAL         BAR           0.0000

            *** ZONE RESULTS ***

  TEMPERATURE LEAVING EACH ZONE:

                   HOT
      ------------------------------------------------------------
      |                                |
HOT IN |              LIQ                | HOT OUT
------> |                               |------>
 235.5 |                               |  34.5
      |                                |
COLDOUT |              LIQ               | COLDIN
<------ |                               |<------
  48.9 |                               |  32.2
      |                                |
      ------------------------------------------------------------
                   COLD
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 9

               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX (CONTINUED)

  ZONE HEAT TRANSFER AND AREA:

  ZONE    HEAT DUTY    AREA    LMTD    AVERAGE U    UA
       CAL/SEC     SQM     C     CAL/SEC-SQCM-K CAL/SEC-K
   1   234911.118    27.7014   41.7701   0.0203    5623.9056
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 10

               U-O-S BLOCK SECTION

HEATX COLD-TQCU B3    TQCURV INLET
------------------------------------
  PRESSURE PROFILE:   CONSTANT2
  PRESSURE DROP:     0.0     BAR
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

-----------------------------------------------------
! DUTY   ! PRES   ! TEMP   ! VFRAC   !
!      !      !      !      !
!      !      !      !      !
!      !      !      !      !
! CAL/SEC  ! BAR    ! C     !      !
```

```
!      !      !      !      !
!============!============!============!============!
!   0.0  !   1.0000 !  48.8889 !   0.0  !
! 1.1186+04 !   1.0000 !  48.0951 !   0.0  !
! 2.2372+04 !   1.0000 !  47.3013 !   0.0  !
! 3.3559+04 !   1.0000 !  46.5075 !   0.0  !
! 4.4745+04 !   1.0000 !  45.7137 !   0.0  !
!------------+------------+------------+------------!
! 5.5931+04 !   1.0000 !  44.9199 !   0.0  !
! 6.7117+04 !   1.0000 !  44.1261 !   0.0  !
! 7.8304+04 !   1.0000 !  43.3323 !   0.0  !
! 8.9490+04 !   1.0000 !  42.5385 !   0.0  !
! 1.0068+05 !   1.0000 !  41.7448 !   0.0  !
!------------+------------+------------+------------!
! 1.1186+05 !   1.0000 !  40.9510 !   0.0  !
! 1.2305+05 !   1.0000 !  40.1573 !   0.0  !
! 1.3423+05 !   1.0000 !  39.3636 !   0.0  !
! 1.4542+05 !   1.0000 !  38.5700 !   0.0  !
! 1.5661+05 !   1.0000 !  37.7763 !   0.0  !
!------------+------------+------------+------------!
! 1.6779+05 !   1.0000 !  36.9827 !   0.0  !
! 1.7898+05 !   1.0000 !  36.1892 !   0.0  !
! 1.9017+05 !   1.0000 !  35.3957 !   0.0  !
! 2.0135+05 !   1.0000 !  34.6022 !   0.0  !
! 2.1254+05 !   1.0000 !  33.8088 !   0.0  !
!------------+------------+------------+------------!
! 2.2372+05 !   1.0000 !  33.0155 !   0.0  !
! 2.3491+05 !   1.0000 !  32.2222 !   0.0  !
-------------------------------------------------------
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 11

               U-O-S BLOCK SECTION

HEATX HOT-TQCUR B3    TQCURV INLET
---------------------------------------
  PRESSURE PROFILE:   CONSTANT2
  PRESSURE DROP:     0.0     BAR
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

-------------------------------------------------------
! DUTY   ! PRES   ! TEMP   ! VFRAC   !
!      !      !      !      !
!      !      !      !      !
!      !      !      !      !
! CAL/SEC  ! BAR    ! C     !      !
!      !      !      !      !
!============!============!============!============!
!   0.0  !   1.2000 !  235.4562 !   0.0  !
! 1.1186+04 !   1.2000 !  227.0836 !   0.0  !
! 2.2372+04 !   1.2000 !  218.6217 !   0.0  !
! 3.3559+04 !   1.2000 !  210.0672 !   0.0  !
! 4.4745+04 !   1.2000 !  201.4167 !   0.0  !
!------------+------------+------------+------------!
! 5.5931+04 !   1.2000 !  192.6662 !   0.0  !
! 6.7117+04 !   1.2000 !  183.8115 !   0.0  !
! 7.8304+04 !   1.2000 !  174.8480 !   0.0  !
! 8.9490+04 !   1.2000 !  165.7710 !   0.0  !
! 1.0068+05 !   1.2000 !  156.5751 !   0.0  !
!------------+------------+------------+------------!
! 1.1186+05 !   1.2000 !  147.2546 !   0.0  !
! 1.2305+05 !   1.2000 !  137.8036 !   0.0  !
! 1.3423+05 !   1.2000 !  128.2154 !   0.0  !
! 1.4542+05 !   1.2000 !  118.4831 !   0.0  !
! 1.5661+05 !   1.2000 !  108.5994 !   0.0  !
!------------+------------+------------+------------!
! 1.6779+05 !   1.2000 !  98.5565 !   0.0  !
! 1.7898+05 !   1.2000 !  88.3462 !   0.0  !
! 1.9017+05 !   1.2000 !  77.9600 !   0.0  !
! 2.0135+05 !   1.2000 !  67.3893 !   0.0  !
! 2.1254+05 !   1.2000 !  56.6253 !   0.0  !
!------------+------------+------------+------------!
! 2.2372+05 !   1.2000 !  45.6598 !   0.0  !
```

```
! 2.3491+05 !   1.2000 !  34.4847 !   0.0  !
-----------------------------------------------------

BLOCK: DECANT  MODEL: DECANTER
--------------------------------
  INLET STREAM:     2
  FIRST LIQUID OUTLET:  GLY-2
  SECOND LIQUID OUTLET: FAME-2
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 12

               U-O-S BLOCK SECTION

BLOCK: DECANT  MODEL: DECANTER (CONTINUED)

            *** MASS AND ENERGY BALANCE ***
                   IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      465.361     465.361     0.00000
    MASS(KG/HR  )      77858.3     77858.3    -0.243272E-06
    ENTHALPY(CAL/SEC )   -0.144886E+08  -0.156537E+08  0.744295E-01

            *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   981.479   KG/HR
  TOTAL CO2E PRODUCTION     981.479   KG/HR

             *** INPUT DATA ***

  LIQUID-LIQUID SPLIT, TP SPECIFICATION
  SPECIFIED TEMPERATURE        C             0.0
  SPECIFIED PRESSURE         BAR           1.37895
  CONVERGENCE TOLERANCE ON EQUILIBRIUM            0.10000E-02
  MAXIMUM NO ITERATIONS ON EQUILIBRIUM            60
  EQUILIBRIUM METHOD              EQUATION-SOLVING
  KLL COEFFICIENTS FROM            OPTION SET OR EOS
  KLL BASIS                        MOLE
  KEY COMPONENT(S):    C14:0-ME C16:0-ME C16:1-ME C18:0-ME
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 13

               U-O-S BLOCK SECTION

BLOCK: DECANT  MODEL: DECANTER (CONTINUED)

              *** RESULTS ***

  OUTLET TEMPERATURE   C                 0.0000
  OUTLET PRESSURE     BAR                1.3790
  CALCULATED HEAT DUTY  CAL/SEC             -0.11651E+07
  MOLAR RATIO 1ST LIQUID / TOTAL LIQUID           0.41200

  L1-L2 PHASE EQUILIBRIUM :
   COMP     F       X1      X2      K
   C14:0-ME  0.037040   0.441665-11  0.062994   0.142628+11
   C16:0-ME  0.16257    0.500562-13  0.27649    0.552349+13
   C16:1-ME  0.087334   0.655168-09  0.14853    0.226704+09
   C18:0-ME  0.010748   0.457913-17  0.018279   0.399191+16
   C18:1-ME  0.074615   0.110054-10  0.12690    0.115304+11
   C18:2-ME  0.039673   0.107079-10  0.067472   0.630111+10
   EPA-ME   0.091087   0.192667-12  0.15491    0.804032+12
   DHA-ME   0.0057239   0.351208-14  0.0097346   0.277176+13
   METHA-01  0.36840    0.70306    0.13391    0.19047
   GLYCE-01  0.12280    0.29694    0.00078623  0.0026478

            *** ASSOCIATED UTILITIES ***

 UTILITY ID FOR REFRIGERANT        REFRIG
 RATE OF CONSUMPTION          4.3902+06 KG/HR
 COST                    48.1169 $/HR
 CO2 EQUIVALENT EMISSIONS        981.4785 KG/HR
```

```
BLOCK: FAMES  MODEL: FLASH2
------------------------------
  INLET STREAM:     FAME-2
  OUTLET VAPOR STREAM:  METH2
  OUTLET LIQUID STREAM: CLEANFA
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      273.631     273.631    -0.207738E-15
    MASS(KG/HR  )      68295.9     68295.9     0.00000
    ENTHALPY(CAL/SEC )   -0.109536E+08  -0.848365E+07  -0.225493

          *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   2447.88   KG/HR
  TOTAL CO2E PRODUCTION     2447.88   KG/HR
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 14

               U-O-S BLOCK SECTION

BLOCK: FAMES  MODEL: FLASH2 (CONTINUED)

             *** INPUT DATA ***
  TWO  PHASE TP FLASH
  SPECIFIED TEMPERATURE C                 235.449
  SPECIFIED PRESSURE  BAR                 1.00000
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

             *** RESULTS ***
  OUTLET TEMPERATURE  C                  235.45
  OUTLET PRESSURE    BAR                 1.0000
  HEAT DUTY       CAL/SEC               0.24700E+07
  VAPOR FRACTION                       0.12477



  V-L PHASE EQUILIBRIUM :

   COMP       F(I)      X(I)      Y(I)      K(I)
   C14:0-ME     0.62994E-01  0.69754E-01  0.15573E-01  0.22326
   C16:0-ME     0.27649    0.31118    0.33080E-01  0.10630
   C16:1-ME     0.14853    0.16731    0.16749E-01  0.10010
   C18:0-ME     0.18279E-01  0.20736E-01  0.10459E-02  0.50437E-01
   C18:1-ME     0.12690    0.14398    0.70866E-02  0.49221E-01
   C18:2-ME     0.67472E-01  0.76550E-01  0.37875E-02  0.49477E-01
   EPA-ME      0.15491    0.17663    0.25489E-02  0.14431E-01
   DHA-ME      0.97346E-02  0.11112E-01  0.70364E-04  0.63321E-02
   METHA-01     0.13391    0.22018E-01  0.91886     41.732
   GLYCE-01     0.78623E-03  0.72684E-03  0.12029E-02   1.6549

            *** ASSOCIATED UTILITIES ***

 UTILITY ID FOR STEAM           HPSTEAM
 RATE OF CONSUMPTION          2.1653+04 KG/HR
 COST                    93.0713 $/HR
 CO2 EQUIVALENT EMISSIONS        2447.8825 KG/HR

BLOCK: GLYSEP  MODEL: FLASH2
------------------------------
  INLET STREAM:     GLY-2
  OUTLET VAPOR STREAM:  METHTOP
  OUTLET LIQUID STREAM: PUREGLY
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
```

```
  TOTAL BALANCE
    MOLE(KMOL/HR )      191.730     191.730     0.00000
    MASS(KG/HR  )      9562.39     9562.39     0.00000
    ENTHALPY(CAL/SEC )   -0.470010E+07  -0.407995E+07  -0.131944
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 15

               U-O-S BLOCK SECTION

BLOCK: GLYSEP  MODEL: FLASH2 (CONTINUED)

           *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   614.606   KG/HR
  TOTAL CO2E PRODUCTION     614.606   KG/HR

             *** INPUT DATA ***
  TWO  PHASE TP FLASH
  SPECIFIED TEMPERATURE C                  163.800
  SPECIFIED PRESSURE  BAR                  0.34474
  MAXIMUM NO. ITERATIONS                   30
  CONVERGENCE TOLERANCE                    0.000100000

             *** RESULTS ***
  OUTLET TEMPERATURE  C                   163.80
  OUTLET PRESSURE    BAR                  0.34474
  HEAT DUTY       CAL/SEC                0.62015E+06
  VAPOR FRACTION                        0.74037



  V-L PHASE EQUILIBRIUM :

   COMP       F(I)      X(I)      Y(I)      K(I)
   C14:0-ME     0.44166E-11  0.83450E-16  0.59654E-11   71486.
   C16:0-ME     0.50056E-13  0.84227E-19  0.67610E-13  0.80271E+06
   C16:1-ME     0.65517E-09  0.23234E-12  0.88484E-09   3808.4
   C18:1-ME     0.11005E-10  0.10714E-14  0.14864E-10   13874.
   C18:2-ME     0.10708E-10  0.15362E-14  0.14462E-10   9414.3
   EPA-ME      0.19267E-12  0.97180E-17  0.26023E-12   26778.
   DHA-ME      0.35121E-14  0.26325E-18  0.47436E-14   18020.
   METHA-01     0.70306    0.12706E-01  0.94515     74.385
   GLYCE-01     0.29694    0.98729    0.54848E-01  0.55554E-01

            *** ASSOCIATED UTILITIES ***

 UTILITY ID FOR STEAM           HPSTEAM
 RATE OF CONSUMPTION          5436.5625 KG/HR
 COST                    23.3680 $/HR
 CO2 EQUIVALENT EMISSIONS        614.6059 KG/HR

BLOCK: S1    MODEL: FLASH2
------------------------------
  INLET STREAMS:     FAME-1   GLY-1    MEOH-1
  OUTLET VAPOR STREAM:  1
  OUTLET LIQUID STREAM: 2
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

            *** MASS AND ENERGY BALANCE ***
                   IN       OUT    RELATIVE DIFF.
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 16

               U-O-S BLOCK SECTION

BLOCK: S1    MODEL: FLASH2 (CONTINUED)
  TOTAL BALANCE
    MOLE(KMOL/HR )      465.361     465.361     0.00000
    MASS(KG/HR  )      77858.3     77858.3     0.00000
    ENTHALPY(CAL/SEC )   -0.146555E+08  -0.144886E+08  -0.113857E-01

            *** CO2 EQUIVALENT SUMMARY ***
```

```
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   0.00000   KG/HR
  TOTAL CO2E PRODUCTION     0.00000   KG/HR

            *** INPUT DATA ***
  TWO  PHASE TP FLASH
  SPECIFIED TEMPERATURE C                 90.0000
  SPECIFIED PRESSURE  BAR                50.0000
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

            *** RESULTS ***
  OUTLET TEMPERATURE  C                   90.000
  OUTLET PRESSURE    BAR                  50.000
  HEAT DUTY       CAL/SEC                0.16686E+06
  VAPOR FRACTION                         0.0000



  V-L PHASE EQUILIBRIUM :

   COMP       F(I)      X(I)      Y(I)      K(I)
   C14:0-ME     0.37040E-01  0.37040E-01  0.80481E-03  0.97269E-03
   C16:0-ME     0.16257    0.16257    0.20840E-02  0.57386E-03
   C16:1-ME     0.87334E-01  0.87334E-01  0.24872E-03  0.12749E-03
   C18:0-ME     0.10748E-01  0.10748E-01  0.84590E-04  0.35232E-03
   C18:1-ME     0.74615E-01  0.74615E-01  0.10978E-03  0.65863E-04
   C18:2-ME     0.39673E-01  0.39673E-01  0.58327E-04  0.65815E-04
   EPA-ME      0.91087E-01  0.91087E-01  0.38030E-04  0.18691E-04
   DHA-ME      0.57239E-02  0.57239E-02  0.81540E-06  0.63772E-05
   METHA-01     0.36840    0.36840    0.99337    0.12071
   GLYCE-01     0.12280    0.12280    0.32013E-02  0.11670E-02
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 17

                 STREAM SECTION

1 2 CLEANFA FAME-1 FAME-2
-------------------------

STREAM ID        1     2     CLEANFA  FAME-1   FAME-2
FROM :         S1     S1     FAMES   ----    DECANT
TO  :          ----   DECANT   B1     S1     FAMES

SUBSTREAM: MIXED
PHASE:         MISSING  LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
  C14:0-ME        0.0    17.2371  16.7054  17.2371  17.2371
  C16:0-ME        0.0    75.6548  74.5255  75.6548  75.6548
  C16:1-ME        0.0    40.6420  40.0703  40.6420  40.6421
  C18:0-ME        0.0    5.0018   4.9661   5.0018   5.0018
  C18:1-ME        0.0    34.7227  34.4808  34.7227  34.7227
  C18:2-ME        0.0    18.4624  18.3331  18.4624  18.4624
  EPA-ME         0.0    42.3882  42.3012  42.3882  42.3883
  DHA-ME         0.0    2.6637   2.6613   2.6637   2.6637
  METHA-01        0.0   171.4403   5.2731   0.0    36.6425
  CARBO-01        0.0    0.0    0.0    0.0    0.0
  GLYCE-01        0.0    57.1477   0.1741   0.0    0.2151
  WATER          0.0    0.0    0.0    0.0    0.0
TOTAL FLOW:
  KMOL/HR         0.0   465.3607  239.4908  236.7727  273.6305
  KG/HR          0.0   7.7858+04 6.6550+04 6.7102+04 6.8296+04
  L/MIN          0.0   1555.1502 1471.6344 1275.1808 1224.0647
STATE VARIABLES:
  TEMP  C        MISSING  90.0000  235.4490  90.0000   0.0
  PRES  BAR       50.0000  50.0000   1.0000  50.0000   1.3790
  VFRAC          MISSING   0.0    0.0    0.0    0.0
  LFRAC          MISSING   1.0000   1.0000   1.0000   1.0000
  SFRAC          MISSING   0.0    0.0    0.0    0.0
ENTHALPY:
  CAL/MOL         MISSING -1.1208+05 -1.2013+05 -1.4514+05 -1.4411+05
```

```
  CAL/GM        MISSING -669.9225 -432.2924 -512.1264 -577.3848
  CAL/SEC        MISSING -1.4489+07 -7.9915+06 -9.5458+06 -1.0954+07
ENTROPY:
  CAL/MOL-K       MISSING -203.4122 -275.6691 -336.4489 -330.9417
  CAL/GM-K       MISSING  -1.2158  -0.9920  -1.1872  -1.3259
DENSITY:
  MOL/CC        MISSING 4.9873-03 2.7123-03 3.0946-03 3.7257-03
  GM/CC         MISSING   0.8344   0.7537   0.8770   0.9299
AVG MW         MISSING  167.3075  277.8828  283.4026  249.5918
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 18

                 STREAM SECTION

GLY-1 GLY-2 MEOH-1 METH2 METHTOP
--------------------------------

STREAM ID        GLY-1   GLY-2   MEOH-1   METH2   METHTOP
FROM :          ----    DECANT   ----    FAMES   GLYSEP
TO  :          S1     GLYSEP   S1     ----    ----

SUBSTREAM: MIXED
PHASE:          LIQUID   LIQUID   LIQUID   VAPOR   VAPOR
COMPONENTS: KMOL/HR
  C14:0-ME        0.0   8.4681-10   0.0    0.5317 8.4680-10
  C16:0-ME        0.0   9.5973-12   0.0    1.1293 9.5973-12
  C16:1-ME        0.0   1.2562-07   0.0    0.5718 1.2560-07
  C18:0-ME        0.0   8.7796-16   0.0   3.5706-02   0.0
  C18:1-ME        0.0   2.1101-09   0.0    0.2419 2.1100-09
  C18:2-ME        0.0   2.0530-09   0.0    0.1293 2.0530-09
  EPA-ME         0.0   3.6940-11   0.0   8.7019-02 3.6940-11
  DHA-ME         0.0   6.7337-13   0.0   2.4022-03 6.7336-13
  METHA-01        0.0   134.7977  171.4403  31.3695  134.1652
  CARBO-01        0.0    0.0    0.0    0.0    0.0
  GLYCE-01       57.1477  56.9325   0.0   4.1066-02   7.7857
  WATER         0.0    0.0    0.0    0.0    0.0
TOTAL FLOW:
  KMOL/HR         57.1477  191.7302  171.4403  34.1397  141.9509
  KG/HR        5263.0000 9562.3932 5493.3170 1745.5621 5015.9664
  L/MIN         71.8865  148.9810  128.9372 2.3882+04 2.4858+05
STATE VARIABLES:
  TEMP  C       90.0000   0.0    90.0000  235.4490  163.8000
  PRES  BAR      50.0000   1.3790  50.0000   1.0000   0.3447
  VFRAC         0.0    0.0    0.0    1.0000   1.0000
  LFRAC         1.0000   1.0000   1.0000   0.0    0.0
  SFRAC         0.0    0.0    0.0    0.0    0.0
ENTHALPY:
  CAL/MOL      -1.5402+05 -8.8251+04 -5.5957+04 -5.1902+04 -5.1159+04
  CAL/GM       -1672.3860 -1769.4686 -1746.3537 -1015.1072 -1447.7973
  CAL/SEC      -2.4449+06 -4.7001+06 -2.6648+06 -4.9220+05 -2.0173+06
ENTROPY:
  CAL/MOL-K      -132.5873  -86.5514  -54.6640  -44.8774  -27.5689
  CAL/GM-K       -1.4397  -1.7354  -1.7060  -0.8777  -0.7802
DENSITY:
  MOL/CC       1.3250-02 2.1449-02 2.2161-02 2.3826-05 9.5175-06
  GM/CC         1.2202   1.0698   0.7101 1.2182-03 3.3631-04
AVG MW         92.0947  49.8742  32.0422  51.1300  35.3359
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 19

                 STREAM SECTION

PROD PUREGLY S1 S2 S3
---------------------

STREAM ID        PROD    PUREGLY  S1     S2     S3
FROM :         B2     GLYSEP   B3     ----    B3
TO  :         ----    ----    ----    B3     ----

SUBSTREAM: MIXED
PHASE:          LIQUID   LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
  C14:0-ME       14.7910 4.1541-15   1.9144   0.0    0.0
  C16:0-ME       65.9849 4.1928-18   8.5406   0.0    0.0
```

```
  C16:1-ME       35.4782 1.1566-11   4.5921   0.0    0.0
  C18:0-ME        4.3970   0.0    0.5691   0.0    0.0
  C18:1-ME       30.5293 5.3333-14   3.9515   0.0    0.0
  C18:2-ME       16.2321 7.6472-14   2.1010   0.0    0.0
  EPA-ME        37.4535 4.8375-16   4.8477   0.0    0.0
  DHA-ME         2.3563 1.3104-17   0.3050   0.0    0.0
  METHA-01        4.6688   0.6325   0.6043   0.0    0.0
  CARBO-01        0.0    0.0    0.0    0.0    0.0
  GLYCE-01        0.1541  49.1468 1.9949-02   0.0    0.0
  WATER         0.0    0.0    0.0   2442.3711 2442.3711
TOTAL FLOW:
  KMOL/HR       212.0452  49.7793  27.4456 2442.3711 2442.3711
  KG/HR        5.8924+04 4546.4268 7626.6736 4.4000+04 4.4000+04
  L/MIN        1302.9965  65.6208  138.5898  743.0201  755.5421
STATE VARIABLES:
  TEMP  C       235.4562  163.8000  34.4846  32.2222  48.8889
  PRES  BAR       1.2000   0.3447   1.2000   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:
  CAL/MOL      -1.2012+05 -1.4917+05 -1.5094+05 -6.8887+04 -6.8541+04
  CAL/GM       -432.2832 -1633.3067 -543.1677 -3823.8310 -3804.6110
  CAL/SEC      -7.0755+06 -2.0627+06 -1.1507+06 -4.6736+07 -4.6501+07
ENTROPY:
  CAL/MOL-K      -275.6689 -122.1902 -351.7763  -40.4127  -39.3087
  CAL/GM-K       -0.9920  -1.3379  -1.2659  -2.2432  -2.1820
DENSITY:
  MOL/CC       2.7123-03 1.2643-02 3.3006-03 5.4785-02 5.3877-02
  GM/CC         0.7537   1.1547   0.9172   0.9870   0.9706
AVG MW         277.8828  91.3317  277.8828  18.0153  18.0153
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                STREAM SECTION

S4 TOLLE
--------

STREAM ID        S4     TOLLE
FROM :         B1     B2
TO  :         B2     B3

SUBSTREAM: MIXED
PHASE:         LIQUID   LIQUID
COMPONENTS: KMOL/HR
  C14:0-ME       16.7054   1.9144
  C16:0-ME       74.5255   8.5406
  C16:1-ME       40.0703   4.5921
  C18:0-ME        4.9661   0.5691
  C18:1-ME       34.4808   3.9515
  C18:2-ME       18.3331   2.1010
  EPA-ME        42.3012   4.8477
  DHA-ME         2.6613   0.3050
  METHA-01        5.2731   0.6043
  CARBO-01        0.0    0.0
  GLYCE-01        0.1741 1.9949-02
  WATER         0.0    0.0
TOTAL FLOW:
  KMOL/HR       239.4908  27.4456
  KG/HR        6.6550+04 7626.6736
  L/MIN        1471.6473  168.6508
STATE VARIABLES:
  TEMP  C       235.4562  235.4562
  PRES  BAR       1.2000   1.2000
  VFRAC         0.0    0.0
  LFRAC         1.0000   1.0000
  SFRAC         0.0    0.0
ENTHALPY:
  CAL/MOL      -1.2012+05 -1.2012+05
  CAL/GM       -432.2832 -432.2832
  CAL/SEC      -7.9913+06 -9.1580+05
ENTROPY:
```

```
  CAL/MOL-K      -275.6689 -275.6689
  CAL/GM-K       -0.9920  -0.9920
DENSITY:
  MOL/CC       2.7123-03 2.7123-03
  GM/CC         0.7537   0.7537
AVG MW         277.8828  277.8828
```


UTILITY SECTION

UTILITY USAGE: HPSTEAM (STEAM)

HIGH PRESSURE STEAM, INLET TEMP=250 C, OUTLET TEMP=249 C, PRES=572 PSIA
INPUT DATA:

INLET TEMPERATURE	250.0000 C
OUTLET TEMPERATURE	249.0000 C
INLET VAPOR FRACTION	1.0000
OUTLET VAPOR FRACTION	0.0
HEAT TRANSFER COEFFICIENT	0.1433 CAL/SEC-SQCM-K
CO2 DATA SOURCE	US-EPA-RULE-E9-5711
CO2 FUEL SOURCE	NATURAL_GAS
CO2 EMISSION FACTOR	2.3400-07 KG/CAL
THERMAL EFFICIENCY	0.8500
PRICE	1.0467-08 $/CAL
INDEX TYPE	FUEL

RESULT:

HEATING VALUE	410.6534 CAL/GM
INDEXED PRICE	1.0467-08 $/CAL
CO2 EMISSION FACTOR	2.3400-07 KG/CAL
TOTAL CO2 EMISSIONS	3062.4884 KG/HR

THIS UTILITY IS PURCHASED

USAGE:

BLOCK	ID	MODEL	DUTY CAL/SEC	USAGE RATE KG/HR	COST $/HR	CO2E EMISSIONS KG/HR
FAMES		FLASH2	2.4700+06	2.1653+04	93.0713	2447.8825
GLYSEP		FLASH2	6.2015+05	5436.5625	23.3680	614.6059
	TOTAL:		3.0901+06	2.7090+04	116.4393	3062.4884

UTILITY SECTION

UTILITY USAGE: REFRIG (REFRIGERANT)

REFRIGERANT 1, INLET TEMP=-25 C, OUTLET TEMP=-24 C
INPUT DATA:

INLET TEMPERATURE	-25.0000 C
OUTLET TEMPERATURE	-24.0000 C
HEAT TRANSFER COEFFICIENT	3.1050-02 CAL/SEC-SQCM-K
CO2 DATA SOURCE	US-EPA-RULE-E9-5711
CO2 FUEL SOURCE	NATURAL_GAS
CO2 EMISSION FACTOR	2.3400-07 KG/CAL
THERMAL EFFICIENCY	1.0000
COOLING VALUE	0.9554 CAL/GM
PRICE	1.1472-08 $/CAL
INDEX TYPE	FUEL

RESULT:

```
  COOLING VALUE             0.9554 CAL/GM
  INDEXED PRICE            1.1472-08 $/CAL
  CO2 EMISSION FACTOR         2.3400-07 KG/CAL
  TOTAL CO2 EMISSIONS         981.4785 KG/HR

 THIS UTILITY IS PURCHASED

 USAGE:

 BLOCK ID MODEL     DUTY        USAGE RATE    COST        CO2E EMISSIONS
             CAL/SEC      KG/HR        $/HR        KG/HR
 -------- ------------ ---------------- ---------------- ---------------- ------------
----
 DECANT  DECANTER       1.1651+06     4.3902+06      48.1169     981.4785
             ---------------- ---------------- ---------------- ----------------
          TOTAL:     1.1651+06     4.3902+06      48.1169     981.4785
             ================ ================ ================ ================

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               PROBLEM STATUS SECTION

BLOCK STATUS
------------

*******************************************************************************
*                                       *
* Calculations were completed normally                  *
*                                       *
* All Unit Operation blocks were completed normally           *
*                                       *
* All streams were flashed normally                    *
*                                       *
* All Utility blocks were completed normally                *
*                                       *
* Properties estimation was completed normally               *
*                                       *
*******************************************************************************
```

25.4.2 Aspen Flowsheet and Report for Hexene Flash and Heat Exchanger

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+ +           ASPEN PLUS CALCULATION REPORT           + +
+ +                                    + +
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ASPEN TECHNOLOGY, INC.         U.S.A. 888/996-7100
781/221-6400              EUROPE (44) 1189-226555

PLATFORM: WINDOWS                    APRIL 13, 2019
VERSION: 36.0  Build 250 Patchlevel 1         SATURDAY
INSTALLATION:                       11:55:41 A.M.

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                RUN CONTROL SECTION
```

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

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TYPE OF RUN: EDIT

INPUT FILE NAME: _0842mwj.inm

INPUT PROBLEM DATA FILE NAME : _0842mwj
OUTPUT PROBLEM DATA FILE NAME: _5439myn
LOCATED IN:


PDF SIZE USED FOR INPUT TRANSLATION:
  NUMBER OF FILE RECORDS (PSIZE) =   0
  NUMBER OF IN-CORE RECORDS   =  256
PSIZE NEEDED FOR SIMULATION  =   1

CALLING PROGRAM NAME:     apmain
LOCATED IN: C:\Program Files (x86)\AspenTech\Aspen Plus V10.0\Engine\\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 2

                FLOWSHEET SECTION

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

  STREAM   SOURCE   DEST      STREAM   SOURCE   DEST
  IN     ----    B1       S2     ----    B3
  HEXENE   B1     B3       OMEGA3   B1     ----
  S1     B3     ----      S3     B3     ----

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

  BLOCK    INLETS            OUTLETS
  B1      IN               HEXENE OMEGA3
  B3      HEXENE S2           S1 S3

CONVERGENCE STATUS SUMMARY
--------------------------

  DESIGN-SPEC SUMMARY
  ===================


  DESIGN                                CONV
  SPEC   ERROR    TOLERANCE  ERR/TOL   VARIABLE  STAT BLOCK
  ------  -----    ---------  -------   --------  ---- -----
  B2    0.16159E-02 0.50000E-02 0.32319    106.92   #  $OLVER02

  # = CONVERGED
  * = NOT CONVERGED
  LB = AT LOWER BOUNDS
  UB = AT UPPER BOUNDS

DESIGN-SPEC: B2
----------------

  SAMPLED VARIABLES:
   METH   : 1-HEX-01MASSFRAC IN STREAM OMEGA3 SUBSTREAM MIXED

  SPECIFICATION:
   MAKE METH APPROACH 0.0100000
   WITHIN     0.0050000

  MANIPULATED VARIABLES:
   VARY   : SENTENCE=PARAM VARIABLE=TEMP IN UOS BLOCK B1
```

```
   LOWER LIMIT =      0.0          C
   UPPER LIMIT =     230.000         C
   FINAL VALUE =     106.917         C

  VALUES OF ACCESSED FORTRAN VARIABLES:
   VARIABLE   VALUE AT START   FINAL VALUE   UNITS
            OF LOOP
   --------   --------------   -----------   -----
   METH      0.177697E-01    0.116159E-01
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                FLOWSHEET SECTION

CONVERGENCE BLOCK: $OLVER02
---------------------------
   SPECS: B2
   MAXIT=  30 STEP-SIZE=  1.0000  % OF RANGE
         MAX-STEP=    100.  % OF RANGE
         XTOL=    1.000000E-08
   THE NEW ALGORITHM WAS USED WITH BRACKETING=NO
   METHOD: SECANT    STATUS: CONVERGED
   TOTAL NUMBER OF ITERATIONS:   3

            *** FINAL VALUES ***


VAR# MANIPUL/TEAR-VAR VARIABLE DESCRIPTION               UNIT     VALUE    PREV VALUE
ERR/TOL
---- ---------------- -------------------------         ----------- ------------  ---
---------  ------------
  1 BLOCK-VAR    B1.PARAM.TEMP                C       106.9173    92.3000     0.3232

            *** ITERATION HISTORY ***

   DESIGN-SPEC ID: B2
   ITERATED: SENTENCE=PARAM VARIABLE=TEMP IN UOS BLOCK B1

   ITERATION VARIABLE     ERROR     ERR/TOL
   --------- --------     -----     -------
     1   90.00      0.7770E-02   1.554
     2   92.30      0.6713E-02   1.343
     3   106.9      0.1616E-02   0.3232

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

SEQUENCE USED WAS:
  HPST
  $OLVER02 B1
  (RETURN $OLVER02)
  B3

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

           *** MASS AND ENERGY BALANCE ***
                  IN       OUT    RELATIVE DIFF.
  CONVENTIONAL COMPONENTS (KMOL/HR )
    EPA-ME          4.26080     4.26080    -0.208454E-15
    DHA-ME          0.268059    0.268059    -0.207086E-15
    1-HEX-01         38.0299     38.0299     0.00000
    WATER           1298.34     1298.34     0.00000
  TOTAL BALANCE
    MOLE(KMOL/HR )      1340.90     1340.90     0.00000
    MASS(KG/HR  )      28030.9     28030.9    -0.129784E-15
    ENTHALPY(CAL/SEC )   -0.251085E+08  -0.249843E+08  -0.494902E-02
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                FLOWSHEET SECTION

OVERALL FLOWSHEET BALANCE (CONTINUED)
```

```
          *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   123.152   KG/HR
  TOTAL CO2E PRODUCTION     123.152   KG/HR
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             PHYSICAL PROPERTIES SECTION

COMPONENTS
----------

 ID    TYPE ALIAS     NAME
  EPA-ME  C   C21H32O2-N1  C21H32O2-N1
  DHA-ME  C   C23H34O2    C23H34O2
  1-HEX-01 C   C6H12-3    1-HEXENE
  WATER  C   H2O      WATER
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 6

               U-O-S BLOCK SECTION

BLOCK: B1    MODEL: FLASH2
------------------------------
  INLET STREAM:     IN
  OUTLET VAPOR STREAM:  HEXENE
  OUTLET LIQUID STREAM: OMEGA3
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      42.5587     42.5587     0.00000
    MASS(KG/HR  )      4640.93     4640.93    -0.195972E-15
    ENTHALPY(CAL/SEC )    -264268.    -140006.    -0.470214

          *** CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E       0.00000   KG/HR
  PRODUCT STREAMS CO2E     0.00000   KG/HR
  NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
  UTILITIES CO2E PRODUCTION   123.152   KG/HR
  TOTAL CO2E PRODUCTION     123.152   KG/HR

            *** INPUT DATA ***
  TWO  PHASE TP FLASH
  SPECIFIED TEMPERATURE C                 106.917
  SPECIFIED PRESSURE  BAR                 0.13332
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

             *** RESULTS ***
  OUTLET TEMPERATURE  C                 106.92
  OUTLET PRESSURE    BAR                0.13332
  HEAT DUTY       CAL/SEC              0.12426E+06
  VAPOR FRACTION                       0.88889



  V-L PHASE EQUILIBRIUM :

   COMP       F(I)      X(I)      Y(I)      K(I)
   EPA-ME      0.10012    0.90079    0.31664E-04  0.35151E-04
   DHA-ME      0.62986E-02  0.56684E-01  0.44625E-06  0.78726E-05
   1-HEX-01     0.89359    0.42521E-01  0.99997     23.517

           *** ASSOCIATED UTILITIES ***

 UTILITY ID FOR STEAM           HPST
 RATE OF CONSUMPTION         1089.3520 KG/HR
 COST                    4.6824 $/HR
 CO2 EQUIVALENT EMISSIONS        123.1518 KG/HR
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 7
```

```
               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX
------------------------------
  HOT SIDE:
  ---------
  INLET STREAM:       HEXENE
  OUTLET STREAM:      S1
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:       S2
  OUTLET STREAM:      S3
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )      1336.17     1336.17     0.00000
    MASS(KG/HR  )      26574.1     26574.1     0.00000
    ENTHALPY(CAL/SEC )   -0.249188E+08  -0.249188E+08  0.149497E-15

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

            *** INPUT DATA ***

  FLASH SPECS FOR HOT SIDE:
  TWO  PHASE   FLASH
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

  FLASH SPECS FOR COLD SIDE:
  TWO  PHASE   FLASH
  MAXIMUM NO. ITERATIONS                  30
  CONVERGENCE TOLERANCE                   0.000100000

  FLOW DIRECTION AND SPECIFICATION:
   COUNTERCURRENT  HEAT EXCHANGER
   SPECIFIED HOT OUTLET TEMP
   SPECIFIED VALUE        C            35.0000
   LMTD CORRECTION FACTOR                 1.00000
ASPEN PLUS  PLAT: WINDOWS  VER: 36.0          04/13/2019 PAGE 8

               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX (CONTINUED)

  PRESSURE SPECIFICATION:
   HOT SIDE PRESSURE DROP    BAR           0.0000
   COLD SIDE PRESSURE DROP    BAR           0.0000

  HEAT TRANSFER COEFFICIENT SPECIFICATION:
   HOT LIQUID  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD LIQUID   CAL/SEC-SQCM-K      0.0203
   HOT LIQUID  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
   HOT LIQUID  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
   HOT 2-PHASE  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
   HOT VAPOR   COLD VAPOR    CAL/SEC-SQCM-K      0.0203

            *** OVERALL RESULTS ***

  STREAMS:
          ---------------------------------------
```

```
          |                  |
  HEXENE  ----->|        HOT         |-----> S1
  T= 1.0692D+02 |                    |    T= 3.5000D+01
  P= 1.3332D-01 |                    |    P= 1.3332D-01
  V= 1.0000D+00 |                    |    V= 9.9995D-01
          |                  |
  S3    <-----|        COLD        |<----- S2
  T= 3.5805D+01 |                    |    T= 3.2222D+01
  P= 1.0000D+00 |                    |    P= 1.0000D+00
  V= 0.0000D+00 |                    |    V= 0.0000D+00
          ---------------------------------------

  DUTY AND AREA:
   CALCULATED HEAT DUTY      CAL/SEC       26854.4911
   CALCULATED (REQUIRED) AREA   SQM           6.2768
   ACTUAL EXCHANGER AREA     SQM           6.2768
   PER CENT OVER-DESIGN                   0.0000

  HEAT TRANSFER COEFFICIENT:
   AVERAGE COEFFICIENT (DIRTY)  CAL/SEC-SQCM-K      0.0203
   UA (DIRTY)           CAL/SEC-K       1274.3014

  LOG-MEAN TEMPERATURE DIFFERENCE:
   LMTD CORRECTION FACTOR                 1.0000
   LMTD (CORRECTED)        C             21.0739
   NUMBER OF SHELLS IN SERIES                1

  PRESSURE DROP:
   HOTSIDE, TOTAL         BAR           0.0000
   COLDSIDE, TOTAL        BAR           0.0000
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               U-O-S BLOCK SECTION

BLOCK: B3    MODEL: HEATX (CONTINUED)

             *** ZONE RESULTS ***

  TEMPERATURE LEAVING EACH ZONE:

                   HOT
     ------------------------------------------------------------
     |                              |
HOT IN |              COND              | HOT OUT
------> |                             |------>
 106.9 |                               |  35.0
     |                              |
COLDOUT |              LIQ               | COLDIN
<------ |                             |<------
  35.8 |                               |  32.2
     |                              |
     ------------------------------------------------------------
                   COLD

  ZONE HEAT TRANSFER AND AREA:

  ZONE    HEAT DUTY    AREA    LMTD    AVERAGE U    UA
       CAL/SEC     SQM     C     CAL/SEC-SQCM-K CAL/SEC-K
   1   26854.491     6.2768   21.0739   0.0203    1274.3014
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               U-O-S BLOCK SECTION

HEATX COLD-TQCU B3    TQCURV INLET
---------------------------------------
  PRESSURE PROFILE:   CONSTANT2
  PRESSURE DROP:     0.0     BAR
  PROPERTY OPTION SET:  RK-SOAVE STANDARD RKS EQUATION OF STATE

-----------------------------------------------------
! DUTY   ! PRES   ! TEMP   ! VFRAC   !
!      !      !      !      !
```

DUTY	PRES	TEMP	VFRAC
CAL/SEC	BAR	C	
0.0	1.0000	35.8051	0.0
1278.7853	1.0000	35.6345	0.0
2557.5706	1.0000	35.6345	0.0
3836.3559	1.0000	35.4639	0.0
5115.1412	1.0000	35.2932	0.0
6393.9264	1.0000	35.1226	0.0
7672.7117	1.0000	34.9520	0.0
8951.4970	1.0000	34.7813	0.0
1.0230+04	1.0000	34.6107	0.0
1.1509+04	1.0000	34.4401	0.0
1.2788+04	1.0000	34.2695	0.0
1.4067+04	1.0000	34.0988	0.0
1.5345+04	1.0000	33.9282	0.0
1.6624+04	1.0000	33.7576	0.0
1.7903+04	1.0000	33.5870	0.0
1.9182+04	1.0000	33.4164	0.0
2.0461+04	1.0000	33.2458	0.0
2.1739+04	1.0000	33.0752	0.0
2.3018+04	1.0000	32.9046	0.0
2.4297+04	1.0000	32.7340	0.0
2.5576+04	1.0000	32.5634	0.0
2.6854+04	1.0000	32.3928	0.0

U-O-S BLOCK SECTION

HEATX HOT-TQCUR B3 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: RK-SOAVE STANDARD RKS EQUATION OF STATE

DUTY	PRES	TEMP	VFRAC
CAL/SEC	BAR	C	
0.0	0.1333	106.9173	1.0000
1278.7853	0.1333	103.7473	1.0000
2557.5706	0.1333	100.5548	1.0000
3836.3559	0.1333	97.3393	1.0000
5115.1412	0.1333	94.1005	1.0000
6393.9264	0.1333	90.8380	1.0000
7672.7117	0.1333	87.5514	1.0000
8951.4970	0.1333	84.2401	1.0000
1.0230+04	0.1333	80.9039	1.0000
1.1509+04	0.1333	77.5421	1.0000
1.2788+04	0.1333	74.1543	1.0000
1.4067+04	0.1333	70.7399	1.0000
1.5345+04	0.1333	67.2982	1.0000
1.6624+04	0.1333	63.8288	1.0000
1.7903+04	0.1333	60.3311	1.0000
1.9182+04	0.1333	56.8043	1.0000
2.0461+04	0.1333	53.2479	1.0000
2.1739+04	0.1333	49.6613	1.0000
2.3018+04	0.1333	46.0438	1.0000

```
! 2.4297+04 !   0.1333 !  42.3948 !   1.0000 !
!------------+------------+------------+------------!
! 2.5576+04 !   0.1333 !  38.7137 !   1.0000 !
! 2.6854+04 !   0.1333 !  35.0000 !   0.9999 !
-----------------------------------------------------
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                 STREAM SECTION

HEXENE IN OMEGA3 S1 S2
----------------------

STREAM ID        HEXENE   IN     OMEGA3   S1     S2
FROM :         B1     ----    B1     B3     ----
TO  :         B3     B1     ----    ----    B3

SUBSTREAM: MIXED
PHASE:         VAPOR   LIQUID   LIQUID   MIXED   LIQUID
COMPONENTS: KMOL/HR
  EPA-ME       1.1978-03   4.2608   4.2596 1.1978-03   0.0
  DHA-ME       1.6882-05   0.2681   0.2680 1.6882-05   0.0
  1-HEX-01       37.8288  38.0299   0.2011  37.8288   0.0
  WATER         0.0    0.0    0.0    0.0   1298.3423
TOTAL FLOW:
  KMOL/HR        37.8300  42.5587   4.7287  37.8300 1298.3423
  KG/HR        3184.1069 4640.9344 1456.8275 3184.1069 2.3390+04
  L/MIN        1.4893+05  110.0547  22.4931 1.2040+05  394.9828
STATE VARIABLES:
  TEMP  C       106.9173  25.0000  106.9173  35.0000  32.2222
  PRES  BAR       0.1333   0.9653   0.1333   0.1333   1.0000
  VFRAC         1.0000   0.0    0.0    0.9999   0.0
  LFRAC         0.0    1.0000   1.0000 5.0550-05   1.0000
  SFRAC         0.0    0.0    0.0    0.0    0.0
ENTHALPY:
  CAL/MOL      -7087.9018 -2.2354+04 -4.9883+04 -9643.4417 -6.8887+04
  CAL/GM        -84.2106 -204.9946 -161.9166 -114.5727 -3823.8310
  CAL/SEC      -7.4482+04 -2.6427+05 -6.5523+04 -1.0134+05 -2.4844+07
ENTROPY:
  CAL/MOL-K      -90.5802 -129.2822 -131.7478  -98.0124  -40.4127
  CAL/GM-K       -1.0762  -1.1856  -0.4276  -1.1645  -2.2432
DENSITY:
  MOL/CC       4.2337-06 6.4451-03 3.5038-03 5.2369-06 5.4785-02
  GM/CC        3.5634-04   0.7028   1.0795 4.4078-04   0.9870
AVG MW         84.1688  109.0477  308.0811  84.1688  18.0153
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                 STREAM SECTION

S3
--

STREAM ID        S3
FROM :         B3
TO  :         ----

SUBSTREAM: MIXED
PHASE:         LIQUID
COMPONENTS: KMOL/HR
  EPA-ME         0.0
  DHA-ME         0.0
  1-HEX-01        0.0
  WATER        1298.3423
TOTAL FLOW:
  KMOL/HR       1298.3423
  KG/HR        2.3390+04
  L/MIN        396.3846
STATE VARIABLES:
  TEMP  C       35.8051
  PRES  BAR       1.0000
  VFRAC         0.0
  LFRAC         1.0000
  SFRAC         0.0
```

```
ENTHALPY:
  CAL/MOL       -6.8813+04
  CAL/GM        -3819.6978
  CAL/SEC       -2.4817+07
ENTROPY:
  CAL/MOL-K       -40.1703
  CAL/GM-K        -2.2298
DENSITY:
  MOL/CC        5.4591-02
  GM/CC          0.9835
AVG MW          18.0153
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                UTILITY SECTION

UTILITY USAGE: HPST   (STEAM)
--------------------------------

HIGH PRESSURE STEAM, INLET TEMP=250 C, OUTLET TEMP=249 C, PRES=572 PSIA
 INPUT DATA:

  INLET TEMPERATURE          250.0000 C
  OUTLET TEMPERATURE          249.0000 C
  INLET VAPOR FRACTION          1.0000
  OUTLET VAPOR FRACTION         0.0
  HEAT TRANSFER COEFFICIENT       0.1433 CAL/SEC-SQCM-K
  CO2 DATA SOURCE              US-EPA-RULE-E9-5711
  CO2 FUEL SOURCE              NATURAL_GAS
  CO2 EMISSION FACTOR         2.3400-07 KG/CAL
  THERMAL EFFICIENCY           0.8500
  PRICE                1.0467-08 $/CAL
  INDEX TYPE                FUEL

 RESULT:

  HEATING VALUE            410.6534 CAL/GM
  INDEXED PRICE            1.0467-08 $/CAL
  CO2 EMISSION FACTOR         2.3400-07 KG/CAL
  TOTAL CO2 EMISSIONS         123.1518 KG/HR

 THIS UTILITY IS PURCHASED

 USAGE:

 BLOCK ID MODEL     DUTY        USAGE RATE    COST        CO2E EMISSIONS
             CAL/SEC      KG/HR        $/HR        KG/HR
 -------- ------------ ---------------- ---------------- ---------------- ------------
----
 B1    FLASH2         1.2426+05     1089.3520      4.6824     123.1518
              ---------------- ---------------- ---------------- ----------------
          TOTAL:     1.2426+05     1089.3520      4.6824     123.1518
              ================ ================ ================ ================

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               PROBLEM STATUS SECTION

BLOCK STATUS
------------

*******************************************************************************
*                                      *
* Calculations were completed normally                  *
*                                      *
* All Unit Operation blocks were completed normally           *
*                                      *
* All streams were flashed normally                    *
*                                      *
* All Utility blocks were completed normally                *
*                                      *
* All Convergence blocks were completed normally              *
*                                      *
```

****

25.4.3 Aspen Flowsheet and Report for Reactors

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+ +           ASPEN PLUS CALCULATION REPORT           + +
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781/221-6400              EUROPE (44) 1189-226555

PLATFORM: WINDOWS                    APRIL 21, 2019
VERSION: 36.0  Build 250 Patchlevel 1         SUNDAY
INSTALLATION:                       10:24:46 A.M.


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RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: NEW

INPUT FILE NAME: _1936ygj.inm

OUTPUT PROBLEM DATA FILE NAME: _1936ygj
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 (x86)\AspenTech\Aspen Plus V10.0\Engine\\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
LLE	----	P-LLE	MEOH	----	BASEREAC
NAOH	----	NAOHTANK	NAOH-H2O	----	NAOHTANK
CW-COLD	----	HX-MEOH	HCL-H2O	----	HCLTANK
HCL	----	HCLTANK	NAOH-WAS	----	WASTE
LLE-P	P-LLE	BASEREAC	NAOH-P	P-NAOH	BASEREAC
OFFA	BASEREAC	P-DIST	OFFA-P	P-DIST	DIST
DISTILL	DIST	SPLIT	BOTTOM	DIST	ACIDREAC
NAOH-MIX	NAOHTANK	P-NAOH	MEOH-RC	SPLIT	HX-MEOH
MEOH-TE	SPLIT	----	MEOH-RCT	HX-MEOH	----
CW-HOT	HX-MEOH	----	HCL-MIX	HCLTANK	P-HCL
PRODUCT	ACIDREAC	DECANT	HCL-P	P-HCL	ACIDREAC
OMEGA-3	DECANT	----	AQ	DECANT	WASTE
WASTEH2O	WASTE	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

```
 BLOCK    INLETS             OUTLETS
 P-LLE    LLE              LLE-P
 P-NAOH    NAOH-MIX            NAOH-P
 BASEREAC   LLE-P MEOH NAOH-P       OFFA
 P-DIST    OFFA              OFFA-P
 DIST     OFFA-P             DISTILL BOTTOM
 NAOHTANK   NAOH-H2O NAOH         NAOH-MIX
 SPLIT    DISTILL            MEOH-RC MEOH-TE
 HX-MEOH   MEOH-RC CW-COLD        MEOH-RCT CW-HOT
 HCLTANK   HCL HCL-H2O          HCL-MIX
 ACIDREAC   BOTTOM HCL-P          PRODUCT
 P-HCL    HCL-MIX            HCL-P
 DECANT    PRODUCT            OMEGA-3 AQ
 WASTE    AQ NAOH-WAS          WASTEH2O

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

SEQUENCE USED WAS:
 HCLTANK P-HCL NAOHTANK P-NAOH P-LLE *BASEREAC *P-DIST *DIST SPLIT
 HX-MEOH ACIDREAC DECANT WASTE

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

          *** MASS AND ENERGY BALANCE ***
              IN     OUT    GENERATION  RELATIVE DIFF.
 CONVENTIONAL COMPONENTS
     (KMOL/HR )
  WATER         180.854    188.083    6.33028   -0.478111E-02
  METHA-01       27.1297    31.6513    4.52161   -0.221749E-09
  EPAME         4.25427    0.00000   -4.25427   0.208773E-15
  DHAME        0.267340    0.00000   -0.267340   -0.415285E-15
  OEPA         0.00000   0.438942E-29 -0.780626E-15  0.00000
  ODHA         0.00000   0.438942E-29 -0.585469E-15  0.00000

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               FLOWSHEET SECTION

OVERALL FLOWSHEET BALANCE (CONTINUED)

          *** MASS AND ENERGY BALANCE ***
              IN     OUT    GENERATION  RELATIVE DIFF.
 CONVENTIONAL COMPONENTS
     (KMOL/HR )
  EPA          0.00000    4.25427    4.25427   0.102447E-07
  DHA          0.00000   0.267340   0.267340   0.102377E-07
  SODIU-01       0.00000    0.00000    0.00000    0.00000
  HYDRO-01       0.488089E-10 0.652964E-20 -0.745674E-11 0.847226
  H3O+         5.87557   0.555191E-06 -5.42594   0.765243E-01
  NA+          3.91524    5.87557   -5.42594   -1.25712
  NAOH(S)        1.96033    0.00000    0.00000    1.00000
  NAOH:(S)       0.00000    0.00000    0.00000    0.00000
  NACL(S)        0.00000    0.00000    5.42594    0.00000
  CL-          5.87557    5.87557   -5.42594   -0.923476
  OH-          3.91524   0.555199E-06 -5.42594   -0.385852
  1-HEX-01       0.310478E-01 0.310478E-01  0.00000   -0.465486E-09
 TOTAL BALANCE
 MOLE(KMOL/HR )      234.078    236.038   -5.42594   -0.312927E-01
 MASS(KG/HR  )      6123.10    6123.10          0.236472E-08
 ENTHALPY(CAL/SEC )  -0.426978E+07 -0.429531E+07        0.594246E-02

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

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```

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
WATER	C	H2O	WATER
METHA-01	C	CH4O	METHANOL
EPAME	C	C21H32O2-N1	C21H32O2-N1
DHAME	C	C23H34O2	C23H34O2
OEPA	C	C20H30O2	MISSING
ODHA	C	C22H32O2	MISSING
EPA	C	C20H30O2-N2	CIS-EICOSAPENTAENOIC-ACID
DHA	C	C22H32O2	DOCOSAHEXAENOIC-ACID
SODIU-01	C	NAOH	SODIUM-HYDROXIDE
HYDRO-01	C	HCL	HYDROGEN-CHLORIDE
H3O+	C	H3O+	H3O+
NA+	C	NA+	NA+
NAOH(S)	C	NAOH	SODIUM-HYDROXIDE
NAOH:(S)	C	NAOH*W	NAOH*H2O
NACL(S)	C	NACL	SODIUM-CHLORIDE
CL-	C	CL-	CL-
OH-	C	OH-	OH-
1-HEX-01	C	C6H12-3	1-HEXENE

LISTID	SUPERCRITICAL COMPONENT LIST
GLOBAL	HYDRO-01

PROPERTY CONSTANT ESTIMATION SECTION

PURE COMPONENT PARAMETERS

COMPONENT ID: OEPA FORMULA: C20H30O2

PROPERTY NAME	PARAMETER NAME	ESTIMATED VALUE	UNITS	METHOD OF ESTIMATION
PARACHOR	PARC	779.30		PARACHOR

PROPERTY CONSTANT ESTIMATION SECTION

PURE COMPONENT PARAMETERS (CONTINUED)

COMPONENT ID: ODHA FORMULA: C22H32O2

PROPERTY NAME	PARAMETER NAME	ESTIMATED VALUE	UNITS	METHOD OF ESTIMATION
PARACHOR	PARC	845.30		PARACHOR

PROPERTY CONSTANT ESTIMATION SECTION

PURE COMPONENT PARAMETERS (CONTINUED)

COMPONENT ID: H3O+ FORMULA: H3O+

```
                PARAMETER  ESTIMATED        METHOD OF
  PROPERTY NAME        NAME     VALUE    UNITS    ESTIMATION
  -------------        -------  ---------  -----    ----------
  FORMATION GIBBS ENERGY  DGAQHG   -0.23713E+09 J/KMOL   AQU-DATA
   FOR HELGESON'S MODEL
  FORMATION ENTHALPY    DHAQHG   -0.28583E+09 J/KMOL   AQU-DATA
   FOR HELGESON'S MODEL
  ABSOLUTE ENTROPY FOR   S25HG     69910.   J/KMOL-K  AQU-DATA
   HELGESON'S MODEL
  BORN COEFFICIENT FOR   OMEGHG    0.12195E+09 J/KMOL   HELGESON
   HELGESON'S MODEL

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          PROPERTY CONSTANT ESTIMATION SECTION

PURE COMPONENT PARAMETERS (CONTINUED)

  --------------------------------
  TEMPERATURE-DEPENDENT PROPERTIES
  --------------------------------
                PARAMETER  PARAMETER        METHOD OF
  PROPERTY NAME        NAME(EL)   VALUES    UNITS    ESTIMATION
  -------------        ---------  ---------  -----    ----------

  HELGESON C1 C2 PARAMETER CHGPAR (1)  81178.   J/KMOL-K  HG-AQU
                   (2) 0.26315E+08


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              U-O-S BLOCK SECTION

BLOCK: ACIDREAC MODEL: RSTOIC
------------------------------
 INLET STREAMS:     BOTTOM   HCL-P
 OUTLET STREAM:     PRODUCT
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
              IN     OUT    GENERATION  RELATIVE DIFF.
 TOTAL BALANCE
 MOLE(KMOL/HR )     98.4596    98.4596   -5.42594   -0.551083E-01
 MASS(KG/HR  )     3199.07    3199.08          -0.722999E-06
 ENTHALPY(CAL/SEC )  -0.176007E+07 -0.180229E+07        0.234284E-01

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

            *** INPUT DATA ***
 STOICHIOMETRY MATRIX:

 REACTION #  1:
  SUBSTREAM MIXED  :
  WATER   -1.00  HYDRO-01 -1.00  H3O+    1.00  CL-    1.00

 REACTION #  2:
  SUBSTREAM MIXED  :
  NA+    -1.00  NACL(S)  1.00  CL-    -1.00

 REACTION #  3:
  SUBSTREAM MIXED  :
  WATER   2.00  H3O+   -1.00  OH-    -1.00

 REACTION #  4:
```

```
  SUBSTREAM MIXED  :
  WATER   1.00  OEPA   -1.00  EPA    1.00  H3O+   -1.00

 REACTION #  5:
  SUBSTREAM MIXED  :
  WATER   1.00  ODHA   -1.00  DHA    1.00  H3O+   -1.00
```



```
              U-O-S BLOCK SECTION

BLOCK: ACIDREAC MODEL: RSTOIC (CONTINUED)
 REACTION CONVERSION SPECS: NUMBER=  5
  REACTION #  1:
  SUBSTREAM:MIXED  KEY COMP:HYDRO-01 CONV FRAC: 1.000
  REACTION #  2:
  SUBSTREAM:MIXED  KEY COMP:NA+   CONV FRAC: 1.000
  REACTION #  3:
  SUBSTREAM:MIXED  KEY COMP:OH-   CONV FRAC: 1.000
  REACTION #  4:
  SUBSTREAM:MIXED  KEY COMP:OEPA   CONV FRAC: 1.000
  REACTION #  5:
  SUBSTREAM:MIXED  KEY COMP:ODHA   CONV FRAC: 1.000



 THREE PHASE TP FLASH
 SPECIFIED TEMPERATURE C                  25.0000
 SPECIFIED PRESSURE  BAR                  1.20000
 MAXIMUM NO. ITERATIONS                   30
 CONVERGENCE TOLERANCE                    0.000100000
 SIMULTANEOUS REACTIONS
 GENERATE COMBUSTION REACTIONS FOR FEED SPECIES     NO

            *** RESULTS ***
 OUTLET TEMPERATURE  C                  25.000
 OUTLET PRESSURE    BAR                  1.2000
 HEAT DUTY       CAL/SEC                -42223.
 VAPOR FRACTION                        0.0000
 1ST LIQUID/TOTAL LIQUID                   1.0000

 REACTION EXTENTS:

  REACTION     REACTION
  NUMBER       EXTENT
           KMOL/HR
  1          0.74567E-11
  2          5.4259
  3          0.90433
  4          4.2543
  5          0.26734
```



```
              U-O-S BLOCK SECTION

BLOCK: ACIDREAC MODEL: RSTOIC (CONTINUED)

 V-L1-L2 PHASE EQUILIBRIUM :

  COMP      F(I)   X1(I)   X2(I)   Y(I)   K1(I)   K2(I)
  WATER     0.936   0.833   0.936   0.936
  METHA-01   0.181E-02 0.161E-02 0.181E-02 0.181E-02
  EPA       0.486E-01 0.432E-01 0.486E-01 0.486E-01
  DHA       0.305E-02 0.272E-02 0.305E-02 0.305E-02
  HYDRO-01    0.00   0.496E-15 0.00   0.00
  H3O+      0.513E-02 0.457E-02 0.513E-02 0.00
  NA+       0.00   0.551E-01 0.00   0.00
  CL-       0.513E-02 0.597E-01 0.513E-02 0.00
```

```
  OH-      0.00   0.985E-16 0.00   0.00
  1-HEX-01   0.144E-04 0.128E-04 0.144E-04 0.144E-04

BLOCK: BASEREAC MODEL: RSTOIC
------------------------------
 INLET STREAMS:     LLE-P    MEOH    NAOH-P
 OUTLET STREAM:     OFFA
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES


  **************************************************************************
  *                                    *
  *   AT LEAST ONE OF THE INLET OR OUTLET STREAMS           *
  *   IS NOT IN CHARGE BALANCE                      *
  *                                    *
  **************************************************************************


          *** MASS AND ENERGY BALANCE ***
              IN     OUT    GENERATION  RELATIVE DIFF.
 TOTAL BALANCE
 MOLE(KMOL/HR )     87.7511    87.7511    0.00000    0.00000
 MASS(KG/HR  )     3341.50    3341.50          0.696516E-06
 ENTHALPY(CAL/SEC )  -0.151271E+07 -0.152159E+07        0.583281E-02

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

            *** INPUT DATA ***

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              U-O-S BLOCK SECTION

BLOCK: BASEREAC MODEL: RSTOIC (CONTINUED)
 STOICHIOMETRY MATRIX:

 REACTION #  1:
  SUBSTREAM MIXED  :
  METHA-01  1.00  EPAME   -1.00  OEPA    1.00  OH-    -1.00

 REACTION #  2:
  SUBSTREAM MIXED  :
  METHA-01  1.00  DHAME   -1.00  ODHA    1.00  OH-    -1.00


 REACTION CONVERSION SPECS: NUMBER=  2
  REACTION #  1:
  SUBSTREAM:MIXED  KEY COMP:EPAME  CONV FRAC: 1.000
  REACTION #  2:
  SUBSTREAM:MIXED  KEY COMP:DHAME  CONV FRAC: 1.000



 TWO  PHASE TP FLASH
 SPECIFIED TEMPERATURE C                 65.0000
 SPECIFIED PRESSURE  BAR                 1.01325
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000
 SIMULTANEOUS REACTIONS
 GENERATE COMBUSTION REACTIONS FOR FEED SPECIES     NO

            *** RESULTS ***
 OUTLET TEMPERATURE  C                65.000
 OUTLET PRESSURE    BAR                1.0132
```

```
 HEAT DUTY        CAL/SEC               -8876.2
 VAPOR FRACTION                        0.0000


 REACTION EXTENTS:

  REACTION     REACTION
  NUMBER       EXTENT
             KMOL/HR
  1           4.2543
  2           0.26734

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               U-O-S BLOCK SECTION

BLOCK: BASEREAC MODEL: RSTOIC (CONTINUED)

 V-L PHASE EQUILIBRIUM :

  COMP       F(I)       X(I)       Y(I)       K(I)
  WATER      0.51529     0.51529    0.15319    0.18345
  METHA-01     0.36069    0.36069    0.84596     1.4473
  OEPA       0.48481E-01  0.48481E-01  0.62380E-09  0.79398E-08
  ODHA       0.30466E-02  0.30466E-02  0.78590E-11  0.15918E-08
  H3O+       0.0000    0.27336E-16   0.0000     0.0000
  NA+       0.61833E-01  0.61833E-01   0.0000     0.0000
  OH-       0.10306E-01  0.10306E-01   0.0000     0.0000
  1-HEX-01     0.35382E-03  0.35382E-03  0.85329E-03   1.4882

BLOCK: DECANT  MODEL: SEP
------------------------------
 INLET STREAM:     PRODUCT
 OUTLET STREAMS:    OMEGA-3   AQ
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN        OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      98.4596     98.4596    0.129899E-14
   MASS(KG/HR  )      3199.08     3199.08    0.113720E-14
   ENTHALPY(CAL/SEC )   -0.180229E+07  -0.180231E+07  0.836480E-05

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


            *** INPUT DATA ***

 FLASH SPECS FOR STREAM OMEGA-3
 TWO  PHASE TP FLASH
 PRESSURE DROP     BAR                 0.0
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000

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               U-O-S BLOCK SECTION

BLOCK: DECANT  MODEL: SEP (CONTINUED)

 FLASH SPECS FOR STREAM AQ
 TWO  PHASE TP FLASH
 PRESSURE DROP     BAR                 0.0
 MAXIMUM NO. ITERATIONS                  30
```

```
 CONVERGENCE TOLERANCE                    0.000100000

 FRACTION OF FEED
  SUBSTREAM= MIXED
   STREAM= OMEGA-3  CPT= EPA    FRACTION=     1.00000
                DHA             1.00000


              *** RESULTS ***

 HEAT DUTY       CAL/SEC               -15.076

COMPONENT = WATER
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

COMPONENT = METHA-01
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

COMPONENT = EPA
 STREAM   SUBSTREAM  SPLIT FRACTION
 OMEGA-3  MIXED         1.00000

COMPONENT = DHA
 STREAM   SUBSTREAM  SPLIT FRACTION
 OMEGA-3  MIXED         1.00000

COMPONENT = H3O+
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

COMPONENT = NA+
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

COMPONENT = CL-
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

COMPONENT = 1-HEX-01
 STREAM   SUBSTREAM  SPLIT FRACTION
 AQ     MIXED         1.00000

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              U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC
------------------------------
 INLETS  - OFFA-P  STAGE  9
 OUTLETS - DISTILL STAGE  1
       BOTTOM  STAGE 16
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES


  **************************************************************************
  *                                    *
  *   AT LEAST ONE OF THE INLET OR OUTLET STREAMS           *
  *   IS NOT IN CHARGE BALANCE                    *
  *                                    *
  **************************************************************************


          *** MASS AND ENERGY BALANCE ***
              IN     OUT    GENERATION  RELATIVE DIFF.
 TOTAL BALANCE
 MOLE(KMOL/HR )     87.7511    87.7511   0.828797E-14 -0.161945E-15
 MASS(KG/HR  )     3341.50    3341.50          0.136091E-15
 ENTHALPY(CAL/SEC )  -0.152152E+07 -0.149604E+07        -0.167432E-01
```

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

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              U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)



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

 ****  INPUT PARAMETERS  ****

 NUMBER OF STAGES                     16
 ALGORITHM OPTION                    STANDARD
 INITIALIZATION OPTION                  STANDARD
 HYDRAULIC PARAMETER CALCULATIONS          NO
 INSIDE LOOP CONVERGENCE METHOD           NEWTON
 DESIGN SPECIFICATION METHOD             NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS         100
 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
 MOLAR REFLUX RATIO                     0.85328
 MOLAR DISTILLATE RATE     KMOL/HR         31.6812

 **** REAC-STAGES SPECIFICATIONS ****

 STAGE TO STAGE      REACTIONS/CHEMISTRY ID
  1     16           GLOBAL


   ***** CHEMISTRY PARAGRAPH GLOBAL *****


    **** REACTION PARAMETERS ****

 RXN NO. TYPE     PHASE   CONC.  TEMP APP TO EQUIL  CONVERSION
                 BASIS      C
  1  EQUILIBRIUM LIQUID   MOLE-GAMMA   0.0000
  2  EQUILIBRIUM LIQUID   MOLE-GAMMA   0.0000

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              U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

   ** STOICHIOMETRIC COEFFICIENTS **

 RXN NO.  WATER    METHA-01   OEPA     ODHA     H3O+
  1   -1.000    0.000    0.000    0.000    1.000
  2   -2.000    0.000    0.000    0.000    1.000

 RXN NO.  NA+     OH-     1-HEX-01   NAOH(S)   NAOH:(S)
  1    0.000    0.000    0.000    0.000    0.000
  2    0.000    1.000    0.000    0.000    0.000
```

** COEFFICIENTS OF EQUILIBRIUM CONSTANT EXPRESSION **

RXN NO.	A	B	C	D	E
2	132.90	-13446.	-22.477	0.0000	0.0000

** SALT STOICHIOMETRIC COEFFICIENTS **

SALT-ID	WATER	METHA-01	OEPA	ODHA	H3O+
NAOH(S)	0.000	0.000	0.000	0.000	0.000
NAOH:(S)	1.000	0.000	0.000	0.000	0.000
NACL(S)	0.000	0.000	0.000	0.000	0.000

SALT-ID	NA+	OH-	1-HEX-01	NAOH(S)	NAOH:(S)
NAOH(S)	1.000	1.000	0.000	0.000	0.000
NAOH:(S)	1.000	1.000	0.000	0.000	0.000
NACL(S)	1.000	0.000	0.000	0.000	0.000

** COEFFICIENTS OF K-SALT EXPRESSION **

SALT ID	A	B	C	D	E
NAOH(S)	433.32	-21657.	-63.231	0.0000	0.0000
NACL(S)	-203.59	4381.2	35.875	-0.67216E-01	0.0000

**** PROFILES ****

P-SPEC STAGE 1 PRES, BAR 1.50000

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
COMPONENT:	DISTILL	BOTTOM
WATER	.35034E-02	.99650
METHA-01	.99500	.50001E-02
OEPA	0.0000	1.0000
ODHA	0.0000	1.0000
H3O+	.29340E-02	.99707

U-O-S BLOCK SECTION

BLOCK: DIST MODEL: RADFRAC (CONTINUED)

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
COMPONENT:	DISTILL	BOTTOM
NA+	0.0000	1.0000
OH-	.49012E-13	1.0000
1-HEX-01	.95925	.40749E-01

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	74.9319
BOTTOM STAGE TEMPERATURE	C	127.548
TOP STAGE LIQUID FLOW	KMOL/HR	27.0332
BOTTOM STAGE LIQUID FLOW	KMOL/HR	56.0698
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOILUP VAPOR FLOW	KMOL/HR	58.0934
MOLAR REFLUX RATIO		0.85329
MOLAR BOILUP RATIO		1.03609
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-134,170.

```
 REBOILER DUTY         CAL/SEC       159,646.


 ****  MANIPULATED VARIABLES  ****

                        BOUNDS       CALCULATED
                    LOWER     UPPER     VALUE
 MOLAR DISTILLATE RATE   KMOL/HR   25.000    40.000    31.681
 MOLAR REFLUX RATIO           0.50000    30.000    0.85329

 ****  DESIGN SPECIFICATIONS  ****

NO SPEC-TYPE   QUALIFIERS       UNIT    SPECIFIED   CALCULATED
                             VALUE     VALUE
1 MOLE-RECOV  STREAMS: DISTILL           0.99500    0.99500
         COMPS:  METHA-01
2 MOLE-FRAC   STREAMS: DISTILL           0.99500    0.99500
         COMPS:  METHA-01
             1-HEX-01

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

 BUBBLE POINT          0.77164E-06 STAGE= 9
 COMPONENT MASS BALANCE     0.18622E-09 STAGE= 14 COMP=1-HEX-01
 ENERGY BALANCE         0.31044E-05 STAGE= 9


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              U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

 ****  PROFILES  ****

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

                     ENTHALPY
STAGE TEMPERATURE  PRESSURE       CAL/MOL      HEAT DUTY
   C       BAR      LIQUID    VAPOR    CAL/SEC

 1  74.932    1.5000    -55792.   -47546.   -.13417+06
 2  76.435    1.5689    -55907.   -47565.
 7  83.390    1.6207    -58738.   -48363.
 8  85.481    1.6310    -59505.   -48664.
 9  89.382    1.6413    -61156.   -48913.
10  90.881    1.6517    -61546.   -49121.
11  94.455    1.6620    -62421.   -49716.
15  118.27    1.7034    -65599.   -56326.
16  127.55    1.7137    -64530.   -56737.    .15965+06

STAGE   FLOW RATE         FEED RATE        PRODUCT RATE
     KMOL/HR          KMOL/HR         KMOL/HR
   LIQUID   VAPOR    LIQUID  VAPOR  MIXED   LIQUID  VAPOR
 1 58.71   0.000                   31.6812
 2 27.05   58.71
 7 25.53   57.62
 8 25.03   57.21
 9 119.5   56.71    87.7510
10 118.8   63.47
11 117.3   62.72
15 114.2   58.48
16 56.07   58.09                   56.0698

 **** MASS FLOW PROFILES ****

STAGE   FLOW RATE         FEED RATE        PRODUCT RATE
     KG/HR            KG/HR           KG/HR
   LIQUID   VAPOR    LIQUID  VAPOR  MIXED   LIQUID  VAPOR
 1 1880.   0.000                  1014.4656
 2 860.8   1880.
```

```
 7 719.9   1773.
 8 681.0   1734.
 9 4205.   1695.   3341.4984
10 4126.   1877.
11 3957.   1799.
15 3394.   1114.
16 2327.   1067.                  2327.0328
```


U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

STAGE	FLOW RATE SOLID1 MIX-SALT KMOL/HR	ENTHALPY SOLID1 MIX-SALT CAL/MOL
1	0.0000	0.0000
2	0.0000	0.0000
7	0.0000	0.0000
8	0.0000	0.0000
9	0.0000	0.0000
10	0.0000	0.0000
11	0.0000	0.0000
15	0.0000	0.0000
16	0.0000	0.0000

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

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+
1	0.50001E-02	0.99406	0.10000E-29	0.10000E-29	0.13991E-14
2	0.18955E-01	0.98006	0.10000E-29	0.10000E-29	0.89340E-14
7	0.27731	0.72186	0.17493E-15	0.53442E-18	0.27351E-11
8	0.34713	0.65211	0.33216E-08	0.46335E-10	0.73286E-11
9	0.47204	0.43665	0.35588E-01	0.22364E-02	0.18321E-16
10	0.50784	0.40024	0.35814E-01	0.22505E-02	0.42483E-16
11	0.58777	0.31916	0.36273E-01	0.22794E-02	0.26478E-15
15	0.89104	0.13828E-01	0.37265E-01	0.23417E-02	0.22887E-12
16	0.80361	0.28226E-02	0.75874E-01	0.47680E-02	0.26864E-12

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

STAGE	NA+	OH-	1-HEX-01
1	0.10000E-29	0.13991E-14	0.94007E-03
2	0.10000E-29	0.89340E-14	0.98477E-03
7	0.10000E-29	0.27351E-11	0.82037E-03
8	0.62716E-21	0.73286E-11	0.75728E-03
9	0.45389E-01	0.75650E-02	0.52429E-03
10	0.45677E-01	0.76130E-02	0.56276E-03
11	0.46263E-01	0.77106E-02	0.54074E-03
15	0.47528E-01	0.79214E-02	0.76050E-04
16	0.96771E-01	0.16129E-01	0.22564E-04

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

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+
1	0.12957E-02	0.99781	0.10129E-37	0.21321E-38	0.0000
2	0.50001E-02	0.99406	0.11175E-37	0.23684E-38	0.0000
7	0.93733E-01	0.90535	0.34679E-23	0.23033E-26	0.0000
8	0.12652	0.87259	0.78065E-16	0.23849E-18	0.0000
9	0.15599	0.84315	0.14659E-08	0.20448E-10	0.0000
10	0.17915	0.81989	0.16853E-08	0.23631E-10	0.0000
11	0.24342	0.75553	0.23445E-08	0.33266E-10	0.0000
15	0.92726	0.72462E-01	0.15681E-07	0.23911E-09	0.0000
16	0.97542	0.24451E-01	0.78876E-07	0.12356E-08	0.0000

U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

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

STAGE	NA+	OH-	1-HEX-01

1	0.0000	0.0000	0.89833E-03
2	0.0000	0.0000	0.94007E-03
7	0.0000	0.0000	0.91533E-03
8	0.0000	0.0000	0.88665E-03
9	0.0000	0.0000	0.85940E-03
10	0.0000	0.0000	0.96750E-03
11	0.0000	0.0000	0.10457E-02
15	0.0000	0.0000	0.27568E-03
16	0.0000	0.0000	0.12767E-03

**** K-VALUES ****

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+
1	0.25913	1.0038	0.10129E-07	0.21321E-08	0.0000
2	0.26379	1.0143	0.11175E-07	0.23684E-08	0.0000
7	0.33800	1.2542	0.19824E-07	0.43099E-08	0.0000
8	0.36448	1.3381	0.23502E-07	0.51472E-08	0.0000
9	0.33045	1.9310	0.41190E-07	0.91435E-08	0.0000
10	0.35276	2.0485	0.47059E-07	0.10500E-07	0.0000
11	0.41415	2.3672	0.64636E-07	0.14594E-07	0.0000
15	1.0407	5.2400	0.42079E-06	0.10211E-06	0.0000
16	1.2138	8.6627	0.10396E-05	0.25914E-06	0.0000

**** K-VALUES ****

STAGE	NA+	OH-	1-HEX-01
1	0.0000	0.0000	0.95559
2	0.0000	0.0000	0.95461
7	0.0000	0.0000	1.1158
8	0.0000	0.0000	1.1708
9	0.0000	0.0000	1.6392
10	0.0000	0.0000	1.7192
11	0.0000	0.0000	1.9338
15	0.0000	0.0000	3.6250
16	0.0000	0.0000	5.6583

**** RATES OF GENERATION ****

KMOL/HR

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+	NA+
1	-.1643E-12	0.000	0.000	0.000	0.8214E-13	0.000
2	-.4076E-12	0.000	0.000	0.000	0.2038E-12	0.000
7	-.9476E-10	0.000	0.000	0.000	0.4738E-10	0.000
8	-.2271E-09	0.000	0.000	0.000	0.1136E-09	0.000
9	0.3668E-09	0.000	0.000	0.000	-.1834E-09	0.000
10	-.5713E-14	0.000	0.000	0.000	0.2856E-14	0.000
11	-.5202E-13	0.000	0.000	0.000	0.2601E-13	0.000
15	-.2241E-10	0.000	0.000	0.000	0.1120E-10	0.000
16	0.2213E-10	0.000	0.000	0.000	-.1107E-10	0.000

U-O-S BLOCK SECTION

BLOCK: DIST MODEL: RADFRAC (CONTINUED)

**** RATES OF GENERATION ****

KMOL/HR

STAGE	OH-	1-HEX-01	NAOH(S)	NAOH:(S)
1	0.8214E-13	0.000	0.000	0.000
2	0.2038E-12	0.000	0.000	0.000
7	0.4738E-10	0.000	0.000	0.000
8	0.1136E-09	0.000	0.000	0.000
9	-.1834E-09	0.000	0.000	0.000
10	0.2856E-14	0.000	0.000	0.000
11	0.2601E-13	0.000	0.000	0.000
15	0.1120E-10	0.000	0.000	0.000
16	-.1107E-10	0.000	0.000	0.000

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

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+
1	0.28131E-02	0.99472	0.94141E-29	0.10227E-28	0.83113E-15
2	0.10729E-01	0.98667	0.94713E-29	0.10289E-28	0.53396E-14
7	0.17719	0.82036	0.18703E-14	0.62073E-17	0.18453E-11
8	0.22981	0.76785	0.36795E-07	0.55761E-09	0.51230E-11

9	0.24178	0.39780	0.30502	0.20823E-01	0.99088E-17
10	0.26340	0.36923	0.31082	0.21219E-01	0.23267E-16
11	0.31387	0.30313	0.32411	0.22127E-01	0.14930E-15
15	0.53995	0.14904E-01	0.37786	0.25795E-01	0.14644E-12
16	0.34883	0.21792E-02	0.55111	0.37623E-01	0.12313E-12

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

STAGE	NA+	OH-	1-HEX-01
1	0.71794E-30	0.74310E-15	0.24708E-02
2	0.72230E-30	0.47741E-14	0.26040E-02
7	0.81536E-30	0.16499E-11	0.24488E-02
8	0.52983E-21	0.45804E-11	0.23421E-02
9	0.29668E-01	0.36582E-02	0.12545E-02
10	0.30233E-01	0.37278E-02	0.13636E-02
11	0.31525E-01	0.38872E-02	0.13489E-02
15	0.36752E-01	0.45317E-02	0.21529E-03
16	0.53604E-01	0.66096E-02	0.45756E-04

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

STAGE	WATER	METHA-01	OEPA	ODHA	H3O+
1	0.72783E-03	0.99691	0.95210E-37	0.21771E-37	0.0000
2	0.28131E-02	0.99472	0.10521E-36	0.24222E-37	0.0000
7	0.54870E-01	0.94263	0.33969E-22	0.24510E-25	0.0000
8	0.75192E-01	0.92235	0.77630E-15	0.25765E-17	0.0000
9	0.93989E-01	0.90359	0.14779E-07	0.22397E-09	0.0000
10	0.10911	0.88814	0.17175E-07	0.26163E-09	0.0000
11	0.15289	0.84404	0.24641E-07	0.37983E-09	0.0000
15	0.87690	0.12188	0.24813E-06	0.41105E-08	0.0000
16	0.95676	0.42657E-01	0.12946E-05	0.22031E-07	0.0000

U-O-S BLOCK SECTION

BLOCK: DIST MODEL: RADFRAC (CONTINUED)

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

STAGE	NA+	OH-	1-HEX-01
1	0.0000	0.0000	0.23574E-02
2	0.0000	0.0000	0.24708E-02
7	0.0000	0.0000	0.25032E-02
8	0.0000	0.0000	0.24617E-02
9	0.0000	0.0000	0.24191E-02
10	0.0000	0.0000	0.27528E-02
11	0.0000	0.0000	0.30683E-02
15	0.0000	0.0000	0.12179E-02
16	0.0000	0.0000	0.58504E-03

****
***** 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     74.932      76.435
 2     76.435      77.108
 7     83.390      85.481
 8     85.481      89.382
 9     89.382      90.881
 10     90.881      94.455
 11     94.455      101.20
 15     118.27      127.55
 16     127.55      127.55
```


U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

```
      MASS FLOW        VOLUME FLOW     MOLECULAR WEIGHT
      KG/HR            L/MIN
STAGE LIQUID FROM VAPOR TO  LIQUID FROM VAPOR TO  LIQUID FROM VAPOR TO
 1  1880.1   1880.1   43.297   17777.   32.021   32.021
 2  860.78   1875.2   19.837   17698.   31.828   31.932
 7  719.88   1734.3   16.058   17119.   28.195   30.314
 8  681.01   1695.5   15.020   17054.   27.212   29.899
 9  4204.5   1877.5   88.929   19052.   35.172   29.580
 10  4126.0   1798.9   86.643   18907.   34.733   28.682
 11  3956.8   1629.8   81.631   18705.   33.737   26.624
 15  3394.0   1067.0   60.123   18632.   29.730   18.367
 16  2327.0   0.0000   39.471   0.0000   41.502


       DENSITY          VISCOSITY     SURFACE TENSION
       GM/CC            CP          DYNE/CM
STAGE LIQUID FROM VAPOR TO   LIQUID FROM VAPOR TO   LIQUID FROM
 1 0.72372   0.17627E-02 0.29183   0.11999E-01  17.965
 2 0.72323   0.17659E-02 0.28830   0.12012E-01  18.461
 7 0.74716   0.16885E-02 0.28563   0.12210E-01  29.439
 8 0.75564   0.16569E-02 0.28394   0.12303E-01  32.323
 9 0.78799   0.16424E-02 0.33261   0.12345E-01  39.507
 10 0.79367   0.15858E-02 0.33044   0.12453E-01  40.999
 11 0.80786   0.14521E-02 0.32478   0.12676E-01  44.258
 15 0.94086   0.95444E-03 0.27511   0.13434E-01  54.160
 16 0.98260          0.29867           51.955


   MARANGONI INDEX  FLOW PARAM     QR     REDUCED F-FACTOR
STAGE  DYNE/CM             L/MIN     (GM-L)**.5/MIN
 1          0.49352E-01    878.39      23602.
 2  0.49581     0.22682E-01    875.61      23519.
 7  3.1533     0.19732E-01    814.73      22245.
 8  2.8833     0.18809E-01    799.48      21953.
 9  -3.1223     0.10224      870.72      24417.
 10  1.4914     0.10252      845.97      23809.
 11  3.2594     0.10293      793.76      22541.
 15  0.54017     0.10131      593.73      18203.
 16  -2.2049             0.0000      0.0000
```


U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)

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

```
 ********************
 *** SECTION  1 ***
 ********************

 STARTING STAGE NUMBER                      2
 ENDING STAGE NUMBER                        9
 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

 TRAY SPECIFICATIONS
 -------------------
 TRAY TYPE                            SIEVE
 NUMBER OF PASSES                         1
 TRAY SPACING          METER           0.60960


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

 STAGE WITH MAXIMUM DIAMETER                  9
 COLUMN DIAMETER         METER            0.46900
 DC AREA/COLUMN AREA                      0.100000
 DOWNCOMER VELOCITY       M/SEC            0.085793
 FLOW PATH LENGTH        METER            0.32223
 SIDE DOWNCOMER WIDTH      METER            0.073387
 SIDE WEIR LENGTH        METER            0.34078
 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   TOTAL AREA  ACTIVE AREA  SIDE DC AREA
         METER     SQM      SQM      SQM
     2   0.46900    0.17276   0.13821    0.17276E-01
     3   0.46900    0.17276   0.13821    0.17276E-01
     4   0.46900    0.17276   0.13821    0.17276E-01
     5   0.46900    0.17276   0.13821    0.17276E-01
     6   0.46900    0.17276   0.13821    0.17276E-01
     7   0.46900    0.17276   0.13821    0.17276E-01
     8   0.46900    0.17276   0.13821    0.17276E-01
     9   0.46900    0.17276   0.13821    0.17276E-01

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               U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)


       **** ADDITIONAL SIZING PROFILES ****

    FLOODING              DC BACKUP/
STAGE FACTOR   PRES. DROP DC BACKUP  (TSPC+WHT)
          BAR     METER
 2   76.83   0.9300E-02 0.2491    37.71
 3   76.23   0.9207E-02 0.2462    37.29
 4   75.45   0.9088E-02 0.2424    36.70
 5   74.45   0.8939E-02 0.2373    35.93
 6   73.24   0.8767E-02 0.2310    34.98
 7   71.94   0.8589E-02 0.2243    33.96
```

```
 8   70.78   0.8431E-02 0.2180    33.01
 9   80.00   0.9940E-02 0.2427    36.75

   HEIGHT   DC REL   TR LIQ REL FRA APPR TO
STAGE OVER WEIR  FROTH DENS FROTH DENS SYS LIMIT
   METER
 2  0.2337E-01 0.6062   0.1754    54.69
 3  0.2299E-01 0.6063   0.1759    53.57
 4  0.2241E-01 0.6063   0.1765    51.99
 5  0.2159E-01 0.6065   0.1774    49.98
 6  0.2058E-01 0.6066   0.1784    47.74
 7  0.1953E-01 0.6068   0.1795    45.58
 8  0.1849E-01 0.6070   0.1806    43.79
 9  0.8756E-01 0.6075   0.1730    46.05



 ********************
 *** SECTION  2 ***
 ********************

 STARTING STAGE NUMBER                    10
 ENDING STAGE NUMBER                      15
 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

 TRAY SPECIFICATIONS
 -------------------
 TRAY TYPE                          SIEVE
 NUMBER OF PASSES                       1
 TRAY SPACING          METER          0.60960

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              U-O-S BLOCK SECTION

BLOCK: DIST   MODEL: RADFRAC (CONTINUED)


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

 STAGE WITH MAXIMUM DIAMETER                 10
 COLUMN DIAMETER         METER           0.46356
 DC AREA/COLUMN AREA                    0.100000
 DOWNCOMER VELOCITY       M/SEC           0.085563
 FLOW PATH LENGTH        METER           0.31849
 SIDE DOWNCOMER WIDTH      METER           0.072535
 SIDE WEIR LENGTH        METER           0.33682
 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   TOTAL AREA  ACTIVE AREA  SIDE DC AREA
        METER     SQM      SQM       SQM
    10   0.46356    0.16877   0.13502    0.16877E-01
    11   0.46356    0.16877   0.13502    0.16877E-01
    12   0.46356    0.16877   0.13502    0.16877E-01
    13   0.46356    0.16877   0.13502    0.16877E-01
```

```
    14   0.46356    0.16877   0.13502    0.16877E-01
    15   0.46356    0.16877   0.13502    0.16877E-01


       **** ADDITIONAL SIZING PROFILES ****

   FLOODING              DC BACKUP/
STAGE FACTOR   PRES. DROP DC BACKUP  (TSPC+WHT)
         BAR      METER
10   80.00   0.9932E-02 0.2410    36.50
11   76.19   0.9221E-02 0.2238    33.89
12   70.75   0.8328E-02 0.2019    30.57
13   65.95   0.7704E-02 0.1853    28.06
14   62.73   0.7455E-02 0.1758    26.61
15   61.08   0.7432E-02 0.1707    25.85

   HEIGHT   DC REL   TR LIQ REL FRA APPR TO
STAGE OVER WEIR  FROTH DENS FROTH DENS SYS LIMIT
   METER
10  0.8669E-01 0.6075   0.1731    45.42
11  0.8215E-01 0.6077   0.1768    41.91
12  0.7541E-01 0.6079   0.1833    37.27
13  0.6925E-01 0.6080   0.1902    33.62
14  0.6507E-01 0.6081   0.1946    31.60
15  0.6247E-01 0.6082   0.1963    30.69

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              U-O-S BLOCK SECTION

BLOCK: HCLTANK MODEL: MIXER
------------------------------
 INLET STREAMS:     HCL     HCL-H2O
 OUTLET STREAM:     HCL-MIX
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                  IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      42.3898     42.3898     0.00000
   MASS(KG/HR  )      872.040     872.040    0.130369E-15
   ENTHALPY(CAL/SEC )    -755023.    -755023.    -0.486311E-08

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

            *** INPUT DATA ***
 TWO  PHASE   FLASH
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000
 OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

BLOCK: HX-MEOH MODEL: HEATX
------------------------------
 HOT SIDE:
 ---------
 INLET STREAM:       MEOH-RC
 OUTLET STREAM:      MEOH-RCT
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES
 COLD SIDE:
 ----------
 INLET STREAM:       CW-COLD
 OUTLET STREAM:      CW-HOT
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
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 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

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              U-O-S BLOCK SECTION

BLOCK: HX-MEOH MODEL: HEATX (CONTINUED)

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      131.292     131.292    0.129886E-14
   MASS(KG/HR  )      2747.50     2747.50    0.496539E-15
   ENTHALPY(CAL/SEC )   -0.239265E+07  -0.239265E+07  -0.144273E-11

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

            *** INPUT DATA ***

 FLASH SPECS FOR HOT SIDE:
 TWO  PHASE   FLASH
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000

 FLASH SPECS FOR COLD SIDE:
 TWO  PHASE   FLASH
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000

 FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT  HEAT EXCHANGER
  SPECIFIED HOT OUTLET TEMP
  SPECIFIED VALUE        C            35.0000
  LMTD CORRECTION FACTOR                 1.00000

 PRESSURE SPECIFICATION:
  HOT SIDE PRESSURE DROP    BAR           0.0000
  COLD SIDE PRESSURE DROP    BAR           0.0000

 HEAT TRANSFER COEFFICIENT SPECIFICATION:
  HOT LIQUID  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE  COLD LIQUID   CAL/SEC-SQCM-K      0.0203
  HOT VAPOR   COLD LIQUID   CAL/SEC-SQCM-K      0.0203
  HOT LIQUID  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE  COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
  HOT VAPOR   COLD 2-PHASE   CAL/SEC-SQCM-K      0.0203
  HOT LIQUID  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
  HOT 2-PHASE  COLD VAPOR    CAL/SEC-SQCM-K      0.0203
  HOT VAPOR   COLD VAPOR    CAL/SEC-SQCM-K      0.0203

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              U-O-S BLOCK SECTION

BLOCK: HX-MEOH MODEL: HEATX (CONTINUED)

           *** OVERALL RESULTS ***

 STREAMS:
         ---------------------------------------
         |                     |
 MEOH-RC  ----->|        HOT          |-----> MEOH-RCT
 T= 7.4932D+01 |                     |    T= 3.5000D+01
 P= 1.5000D+00 |                     |    P= 1.5000D+00
 V= 0.0000D+00 |                     |    V= 0.0000D+00
         |                     |
```

```
 CW-HOT  <-----|        COLD        |<----- CW-COLD
 T= 4.8750D+01 |                    |    T= 3.2222D+01
 P= 1.0132D+00 |                    |    P= 1.0132D+00
 V= 0.0000D+00 |                    |    V= 0.0000D+00
         ---------------------------------------

 DUTY AND AREA:
  CALCULATED HEAT DUTY      CAL/SEC        8583.9410
  CALCULATED (REQUIRED) AREA   SQM           4.0529
  ACTUAL EXCHANGER AREA     SQM           4.0529
  PER CENT OVER-DESIGN                    0.0000

 HEAT TRANSFER COEFFICIENT:
  AVERAGE COEFFICIENT (DIRTY)  CAL/SEC-SQCM-K      0.0203
  UA (DIRTY)           CAL/SEC-K       822.8148

 LOG-MEAN TEMPERATURE DIFFERENCE:
  LMTD CORRECTION FACTOR                 1.0000
  LMTD (CORRECTED)        C             10.4324
  NUMBER OF SHELLS IN SERIES                 1

 PRESSURE DROP:
  HOTSIDE, TOTAL         BAR           0.0000
  COLDSIDE, TOTAL        BAR           0.0000

           *** ZONE RESULTS ***

 TEMPERATURE LEAVING EACH ZONE:

                  HOT
    ------------------------------------------------------------
    |                                 |
HOT IN |              LIQ                | HOT OUT
------> |                               |------>
 74.9 |                                 |  35.0
    |                                 |
COLDOUT |               LIQ               | COLDIN
<------ |                               |<------
 48.7 |                                 |  32.2
    |                                 |
    ------------------------------------------------------------
                  COLD
```



```
              U-O-S BLOCK SECTION

BLOCK: HX-MEOH MODEL: HEATX (CONTINUED)

 ZONE HEAT TRANSFER AND AREA:

 ZONE    HEAT DUTY    AREA    LMTD    AVERAGE U    UA
      CAL/SEC     SQM     C     CAL/SEC-SQCM-K CAL/SEC-K
  1    8583.941     4.0529   10.4324   0.0203     822.8148
```



```
              U-O-S BLOCK SECTION

HEATX COLD-TQCU HX-MEOH TQCURV INLET
------------------------------------
 PRESSURE PROFILE:   CONSTANT2
 PRESSURE DROP:     0.0     BAR
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

-----------------------------------------------------
! DUTY   ! PRES   ! TEMP   ! VFRAC   !
!      !      !      !      !
!      !      !      !      !
!      !      !      !      !
```

CAL/SEC	BAR	C		
0.0	1.0133	48.7498	0.0	
408.7591	1.0133	47.9631	0.0	
817.5182	1.0133	47.1763	0.0	
1226.2773	1.0133	46.3895	0.0	
1635.0364	1.0133	45.6026	0.0	
2043.7955	1.0133	44.8157	0.0	
2452.5546	1.0133	44.0288	0.0	
2861.3137	1.0133	43.2418	0.0	
3270.0728	1.0133	42.4548	0.0	
3678.8319	1.0133	41.6678	0.0	
4087.5910	1.0133	40.8807	0.0	
4496.3501	1.0133	40.0937	0.0	
4905.1092	1.0133	39.3066	0.0	
5313.8683	1.0133	38.5195	0.0	
5722.6274	1.0133	37.7324	0.0	
6131.3865	1.0133	36.9452	0.0	
6540.1456	1.0133	36.1581	0.0	
6948.9047	1.0133	35.3709	0.0	
7357.6638	1.0133	34.5837	0.0	
7766.4229	1.0133	33.7966	0.0	
8175.1820	1.0133	33.0094	0.0	
8583.9410	1.0133	32.2222	0.0	

U-O-S BLOCK SECTION

HEATX HOT-TQCUR HX-MEOH TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
HENRY-COMPS ID: GLOBAL
CHEMISTRY ID: GLOBAL - TRUE SPECIES

DUTY	PRES	TEMP	VFRAC	
CAL/SEC	BAR	C		
0.0	1.5000	74.9319	0.0	
408.7591	1.5000	73.1332	0.0	
817.5182	1.5000	71.3158	0.0	
1226.2773	1.5000	69.4932	0.0	
1635.0364	1.5000	67.6609	0.0	
2043.7955	1.5000	65.8188	0.0	
2452.5546	1.5000	63.9669	0.0	
2861.3137	1.5000	62.1053	0.0	
3270.0728	1.5000	60.2338	0.0	
3678.8319	1.5000	58.3524	0.0	
4087.5910	1.5000	56.4611	0.0	
4496.3501	1.5000	54.5598	0.0	
4905.1092	1.5000	52.6485	0.0	
5313.8683	1.5000	50.7272	0.0	
5722.6274	1.5000	48.7956	0.0	
6131.3865	1.5000	46.8491	0.0	
6540.1456	1.5000	44.9063	0.0	
6948.9047	1.5000	42.9454	0.0	

```
! 7357.6638 !   1.5000 !  40.9743 !   0.0  !
! 7766.4229 !   1.5000 !  38.9931 !   0.0  !
!------------+------------+------------+------------!
! 8175.1820 !   1.5000 !  37.0017 !   0.0  !
! 8583.9410 !   1.5000 !  35.0001 !   0.0  !
-------------------------------------------------

BLOCK: NAOHTANK MODEL: MIXER
------------------------------
 INLET STREAMS:     NAOH-H2O  NAOH
 OUTLET STREAM:     NAOH-MIX
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

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              U-O-S BLOCK SECTION

BLOCK: NAOHTANK MODEL: MIXER (CONTINUED)

          *** MASS AND ENERGY BALANCE ***
                   IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      54.1221     55.9324    -0.323661E-01
   MASS(KG/HR  )      1029.16     1029.16     0.00000
   ENTHALPY(CAL/SEC )   -0.101696E+07  -0.101696E+07  -0.880767E-09

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

            *** INPUT DATA ***
 TWO  PHASE   FLASH
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000
 OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

BLOCK: P-DIST  MODEL: PUMP
------------------------------
 INLET STREAM:     OFFA
 OUTLET STREAM:     OFFA-P
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES


  ***************************************************************************
  *                                     *
  *   AT LEAST ONE OF THE INLET OR OUTLET STREAMS           *
  *   IS NOT IN CHARGE BALANCE                      *
  *                                     *
  ***************************************************************************


          *** MASS AND ENERGY BALANCE ***
                   IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      87.7511     87.7511    0.323890E-15
   MASS(KG/HR  )      3341.50     3341.50    -0.136091E-15
   ENTHALPY(CAL/SEC )   -0.152159E+07  -0.152152E+07  -0.471939E-04

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              U-O-S BLOCK SECTION

BLOCK: P-DIST  MODEL: PUMP (CONTINUED)

          *** CO2 EQUIVALENT SUMMARY ***
```

```
 FEED STREAMS CO2E       0.00000   KG/HR
 PRODUCT STREAMS CO2E     0.00000   KG/HR
 NET STREAMS CO2E PRODUCTION  0.00000   KG/HR
 UTILITIES CO2E PRODUCTION   0.00000   KG/HR
 TOTAL CO2E PRODUCTION     0.00000   KG/HR

           *** INPUT DATA ***
 OUTLET PRESSURE BAR                  1.80000
 DRIVER EFFICIENCY                    1.00000

 FLASH SPECIFICATIONS:
 LIQUID PHASE CALCULATION
 NO FLASH PERFORMED
 MAXIMUM NUMBER OF ITERATIONS              30
 TOLERANCE                        0.000100000

            *** RESULTS ***
 VOLUMETRIC FLOW RATE L/MIN             67.7794
 PRESSURE CHANGE BAR                   0.78675
 NPSH AVAILABLE  M-KGF/KG               4.85804
 FLUID POWER KW                        0.088876
 BRAKE POWER KW                        0.30060
 ELECTRICITY KW                        0.30060
 PUMP EFFICIENCY USED                     0.29566
 NET WORK REQUIRED KW                  0.30060
 HEAD DEVELOPED M-KGF/KG                9.76391

BLOCK: P-HCL  MODEL: PUMP
------------------------------
 INLET STREAM:     HCL-MIX
 OUTLET STREAM:     HCL-P
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      42.3898     42.3898    -0.335243E-15
   MASS(KG/HR  )      872.040     872.040    -0.130369E-15
   ENTHALPY(CAL/SEC )    -755023.    -755013.    -0.136359E-04

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              U-O-S BLOCK SECTION

BLOCK: P-HCL  MODEL: PUMP (CONTINUED)

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

           *** INPUT DATA ***
 OUTLET PRESSURE BAR                  1.60000
 DRIVER EFFICIENCY                    1.00000

 FLASH SPECIFICATIONS:
 LIQUID PHASE CALCULATION
 NO FLASH PERFORMED
 MAXIMUM NUMBER OF ITERATIONS              30
 TOLERANCE                        0.000100000

            *** RESULTS ***
 VOLUMETRIC FLOW RATE L/MIN             13.0318
 PRESSURE CHANGE BAR                   0.58675
 NPSH AVAILABLE  M-KGF/KG               8.96052
 FLUID POWER KW                        0.012744
 BRAKE POWER KW                        0.043104
 ELECTRICITY KW                        0.043104
```

```
 PUMP EFFICIENCY USED                    0.29566
 NET WORK REQUIRED KW                    0.043104
 HEAD DEVELOPED M-KGF/KG                   5.36477

BLOCK: P-LLE  MODEL: PUMP
------------------------------
 INLET STREAM:     LLE
 OUTLET STREAM:     LLE-P
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN        OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      4.53861     4.53861     0.00000
   MASS(KG/HR  )      1439.41     1439.41     0.00000
   ENTHALPY(CAL/SEC )    -64295.5    -64266.4    -0.452701E-03

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               U-O-S BLOCK SECTION

BLOCK: P-LLE  MODEL: PUMP (CONTINUED)

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

            *** INPUT DATA ***
 OUTLET PRESSURE BAR                   1.20000
 DRIVER EFFICIENCY                     1.00000

 FLASH SPECIFICATIONS:
 LIQUID PHASE CALCULATION
 NO FLASH PERFORMED
 MAXIMUM NUMBER OF ITERATIONS              30
 TOLERANCE                         0.000100000

             *** RESULTS ***
 VOLUMETRIC FLOW RATE L/MIN              20.2605
 PRESSURE CHANGE BAR                   1.06700
 NPSH AVAILABLE  M-KGF/KG                1.04642
 FLUID POWER KW                        0.036030
 BRAKE POWER KW                        0.12186
 ELECTRICITY KW                        0.12186
 PUMP EFFICIENCY USED                     0.29566
 NET WORK REQUIRED KW                     0.12186
 HEAD DEVELOPED M-KGF/KG                  9.18885

BLOCK: P-NAOH  MODEL: PUMP
------------------------------
 INLET STREAM:     NAOH-MIX
 OUTLET STREAM:     NAOH-P
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN        OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      55.9324     55.9324    0.127036E-15
   MASS(KG/HR  )      1029.16     1029.16    0.220931E-15
   ENTHALPY(CAL/SEC )   -0.101696E+07  -0.101696E+07  -0.373691E-05

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               U-O-S BLOCK SECTION
```

```
BLOCK: P-NAOH  MODEL: PUMP (CONTINUED)

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

            *** INPUT DATA ***
 PRESSURE CHANGE BAR                   0.20000
 DRIVER EFFICIENCY                     1.00000

 FLASH SPECIFICATIONS:
 LIQUID PHASE CALCULATION
 NO FLASH PERFORMED
 MAXIMUM NUMBER OF ITERATIONS              30
 TOLERANCE                        0.000100000

             *** RESULTS ***
 VOLUMETRIC FLOW RATE L/MIN             14.1129
 PRESSURE CHANGE BAR                   0.20000
 NPSH AVAILABLE  M-KGF/KG               7.61171
 FLUID POWER KW                      0.0047043
 BRAKE POWER KW                      0.015911
 ELECTRICITY KW                      0.015911
 PUMP EFFICIENCY USED                   0.29566
 NET WORK REQUIRED KW                   0.015911
 HEAD DEVELOPED M-KGF/KG                1.67800

BLOCK: SPLIT  MODEL: FSPLIT
------------------------------
 INLET STREAM:     DISTILL
 OUTLET STREAMS:    MEOH-RC   MEOH-TE
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN       OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )      31.6812     31.6812     0.00000
   MASS(KG/HR  )      1014.47     1014.47     0.00000
   ENTHALPY(CAL/SEC )    -490986.    -490986.     0.00000

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              U-O-S BLOCK SECTION

BLOCK: SPLIT  MODEL: FSPLIT (CONTINUED)

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

            *** INPUT DATA ***

KEY= 1  SUBSTREAM NO.= 1 CPT.= METHA-01

MOLE-FLOW (KMOL/HR )      STRM=MEOH-RC FLOW=    27.1297   KEY= 1

             *** RESULTS ***

STREAM= MEOH-RC    SPLIT=     0.86145   KEY= 1  STREAM-ORDER=  1
    MEOH-TE            0.13855      0          2

BLOCK: WASTE  MODEL: MIXER
------------------------------
 INLET STREAMS:     AQ     NAOH-WAS
```

```
 OUTLET STREAM:     WASTEH2O
 PROPERTY OPTION SET:  ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
 HENRY-COMPS ID:    GLOBAL
 CHEMISTRY ID:     GLOBAL  - TRUE SPECIES

          *** MASS AND ENERGY BALANCE ***
                 IN        OUT    RELATIVE DIFF.
 TOTAL BALANCE
   MOLE(KMOL/HR )       95.6855     95.8355    -0.156531E-02
   MASS(KG/HR  )       1860.49     1860.49     0.488847E-15
   ENTHALPY(CAL/SEC )   -0.175255E+07  -0.175255E+07  -0.758251E-07

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

            *** INPUT DATA ***
 TWO  PHASE   FLASH
 MAXIMUM NO. ITERATIONS                  30
 CONVERGENCE TOLERANCE                   0.000100000
 OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

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                STREAM SECTION

AQ BOTTOM CW-COLD CW-HOT DISTILL
--------------------------------

STREAM ID        AQ     BOTTOM   CW-COLD  CW-HOT   DISTILL
FROM :         DECANT   DIST    ----    HX-MEOH  DIST
TO  :         WASTE   ACIDREAC  HX-MEOH  ----    SPLIT

SUBSTREAM: MIXED
PHASE:         LIQUID   LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
 WATER         82.0273  45.0584  104.0000  104.0000   0.1584
 METHA-01        0.1583   0.1583   0.0    0.0    31.4930
 EPAME         0.0    0.0    0.0    0.0    0.0
 DHAME         0.0    0.0    0.0    0.0    0.0
 OEPA          0.0    4.2543   0.0    0.0   3.1681-29
 ODHA          0.0    0.2673   0.0    0.0   3.1681-29
 EPA          0.0    0.0    0.0    0.0    0.0
 DHA          0.0    0.0    0.0    0.0    0.0
 SODIU-01        0.0    0.0    0.0    0.0    0.0
 HYDRO-01      1.7212-14   0.0    0.0    0.0    0.0
 H3O+          0.4496 1.5063-11 2.4460-07 4.1896-07 4.4324-14
 NA+          5.4259   5.4259   0.0    0.0   3.1681-29
 NAOH(S)         0.0    0.0    0.0    0.0    0.0
 NAOH:(S)        0.0    0.0    0.0    0.0    0.0
 NACL(S)         0.0    0.0    0.0    0.0    0.0
 CL-          5.8756   0.0    0.0    0.0    0.0
 OH-         2.9307-14   0.9043 2.4460-07 4.1896-07 4.4324-14
 1-HEX-01      1.2652-03 1.2652-03   0.0    0.0   2.9783-02
TOTAL FLOW:
 KMOL/HR        93.9380  56.0698  104.0000  104.0000  31.6812
 KG/HR        1824.5220 2327.0328 1873.5891 1873.5891 1014.4657
 L/MIN         26.9272  39.4709  31.3814  31.5852  23.3623
STATE VARIABLES:
 TEMP  C       25.0000  127.5480  32.2222  48.7498  74.9319
 PRES  BAR       1.2000   1.7137   1.0133   1.0133   1.5000
 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:
 CAL/MOL      -6.5924+04 -6.4530+04 -6.8181+04 -6.7884+04 -5.5792+04
 CAL/GM       -3394.1952 -1554.8526 -3784.6468 -3768.1533 -1742.3468
 CAL/SEC      -1.7202+06 -1.0051+06 -1.9697+06 -1.9611+06 -4.9099+05
ENTROPY:
```

```
 CAL/MOL-K      -35.1817  -50.9154  -38.5405  -37.5929  -53.6483
 CAL/GM-K       -1.8114  -1.2268  -2.1393  -2.0867  -1.6754
DENSITY:
 MOL/CC       5.8143-02 2.3676-02 5.5234-02 5.4878-02 2.2601-02
 GM/CC         1.1293   0.9826   0.9951   0.9886   0.7237
AVG MW         19.4226  41.5024  18.0153  18.0153  32.0210

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                STREAM SECTION

HCL HCL-H2O HCL-MIX HCL-P LLE
-----------------------------

STREAM ID        HCL    HCL-H2O  HCL-MIX  HCL-P   LLE
FROM :          ----    ----    HCLTANK  P-HCL   ----
TO   :         HCLTANK  HCLTANK  P-HCL   ACIDREAC  P-LLE

SUBSTREAM: MIXED
PHASE:          LIQUID   LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
 WATER          21.8710   8.7676  30.6386  30.6386   0.0
 METHA-01         0.0    0.0    0.0    0.0    0.0
 EPAME          0.0    0.0    0.0    0.0    4.2543
 DHAME          0.0    0.0    0.0    0.0    0.2673
 OEPA           0.0    0.0    0.0    0.0    0.0
 ODHA           0.0    0.0    0.0    0.0    0.0
 EPA           0.0    0.0    0.0    0.0    0.0
 DHA           0.0    0.0    0.0    0.0    0.0
 SODIU-01         0.0    0.0    0.0    0.0    0.0
 HYDRO-01       4.8809-11   0.0   7.4593-12 7.4567-12   0.0
 H3O+           5.8756 1.5831-08   5.8756   5.8756   0.0
 NA+           0.0    0.0    0.0    0.0    0.0
 NAOH(S)          0.0    0.0    0.0    0.0    0.0
 NAOH:(S)         0.0    0.0    0.0    0.0    0.0
 NACL(S)          0.0    0.0    0.0    0.0    0.0
 CL-           5.8756   0.0    5.8756   5.8756   0.0
 OH-          1.8816-18 1.5831-08 5.1120-17 5.1348-17   0.0
 1-HEX-01         0.0    0.0    0.0    0.0   1.7000-02
TOTAL FLOW:
 KMOL/HR         33.6221   8.7676  42.3898  42.3898   4.5386
 KG/HR         714.0890  157.9514  872.0404  872.0404 1439.4084
 L/MIN          10.3815   2.6400  13.0318  13.0318  20.2605
STATE VARIABLES:
 TEMP  C        25.0000  25.0000  36.8162  36.8648  107.0000
 PRES  BAR        1.0133   1.0133   1.0133   1.6000   0.1330
 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:
 CAL/MOL       -6.3029+04 -6.8311+04 -6.4121+04 -6.4120+04 -5.0999+04
 CAL/GM        -2967.6340 -3791.8538 -3116.9237 -3116.8812 -160.8048
 CAL/SEC       -5.8865+05 -1.6637+05 -7.5502+05 -7.5501+05 -6.4295+04
ENTROPY:
 CAL/MOL-K       -37.7273  -38.9708  -37.5618  -37.5597 -132.2130
 CAL/GM-K        -1.7764  -2.1632  -1.8259  -1.8258  -0.4169
DENSITY:
 MOL/CC        5.3978-02 5.5351-02 5.4213-02 5.4213-02 3.7335-03
 GM/CC          1.1464   0.9972   1.1153   1.1153   1.1841
AVG MW          21.2387  18.0153  20.5720  20.5720  317.1474

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                STREAM SECTION

LLE-P MEOH MEOH-RC MEOH-RCT MEOH-TE
-----------------------------------

STREAM ID        LLE-P   MEOH    MEOH-RC  MEOH-RCT  MEOH-TE
FROM :          P-LLE   ----    SPLIT   HX-MEOH  SPLIT
TO   :         BASEREAC  BASEREAC  HX-MEOH  ----    ----
```

```
SUBSTREAM: MIXED
PHASE:          LIQUID   LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
 WATER          0.0    0.1363   0.1365   0.1365 2.1948-02
 METHA-01         0.0    27.1297  27.1297  27.1297   4.3633
 EPAME          4.2543   0.0    0.0    0.0    0.0
 DHAME          0.2673   0.0    0.0    0.0    0.0
 OEPA           0.0    0.0   2.7292-29   0.0   4.3894-30
 ODHA           0.0    0.0   2.7292-29   0.0   4.3894-30
 EPA          0.0    0.0    0.0    0.0    0.0
 DHA          0.0    0.0    0.0    0.0    0.0
 SODIU-01         0.0    0.0    0.0    0.0    0.0
 HYDRO-01         0.0    0.0    0.0    0.0    0.0
 H3O+           0.0   1.9731-14 3.8183-14 1.9839-14 6.1410-15
 NA+          0.0    0.0   2.7292-29   0.0   4.3894-30
 NAOH(S)          0.0    0.0    0.0    0.0    0.0
 NAOH:(S)         0.0    0.0    0.0    0.0    0.0
 NACL(S)          0.0    0.0    0.0    0.0    0.0
 CL-            0.0    0.0    0.0    0.0    0.0
 OH-            0.0   1.9731-14 3.8183-14 1.9839-14 6.1410-15
 1-HEX-01       1.7000-02 1.4048-02 2.5656-02 2.5656-02 4.1264-03
TOTAL FLOW:
 KMOL/HR          4.5386  27.2801  27.2918  27.2918   4.3894
 KG/HR         1439.4084  872.9325  873.9119  873.9119  140.5538
 L/MIN           20.2631  18.8084  20.1255  18.8315   3.2368
STATE VARIABLES:
 TEMP  C        107.1361  35.0000  74.9319  35.0000  74.9319
 PRES  BAR        1.2000   1.3000   1.5000   1.5000   1.5000
 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:
 CAL/MOL       -5.0976+04 -5.6941+04 -5.5792+04 -5.6924+04 -5.5792+04
 CAL/GM        -160.7320 -1779.4680 -1742.3468 -1777.7075 -1742.3468
 CAL/SEC       -6.4266+04 -4.3149+05 -4.2296+05 -4.3154+05 -6.8026+04
ENTROPY:
 CAL/MOL-K       -132.1526  -56.8741  -53.6483  -56.8963  -53.6483
 CAL/GM-K        -0.4167  -1.7774  -1.6754  -1.7768  -1.6754
DENSITY:
 MOL/CC        3.7331-03 2.4174-02 2.2601-02 2.4154-02 2.2601-02
 GM/CC          1.1839   0.7735   0.7237   0.7734   0.7237
AVG MW          317.1474  31.9989  32.0210  32.0210  32.0210

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                STREAM SECTION

NAOH NAOH-H2O NAOH-MIX NAOH-P NAOH-WAS
--------------------------------------

STREAM ID         NAOH    NAOH-H2O  NAOH-MIX  NAOH-P   NAOH-WAS
FROM :          ----    ----    NAOHTANK  P-NAOH   ----
TO   :        NAOHTANK  NAOHTANK  P-NAOH   BASEREAC  WASTE

SUBSTREAM: MIXED
PHASE:          MIXED   LIQUID   LIQUID   LIQUID   MIXED
COMPONENTS: KMOL/HR
 WATER          12.0467  33.0338  45.0805  45.0805   0.9983
 METHA-01         0.0    0.0    0.0    0.0    0.0
 EPAME          0.0    0.0    0.0    0.0    0.0
 DHAME          0.0    0.0    0.0    0.0    0.0
 OEPA           0.0    0.0    0.0    0.0    0.0
 ODHA           0.0    0.0    0.0    0.0    0.0
 EPA          0.0    0.0    0.0    0.0    0.0
 DHA          0.0    0.0    0.0    0.0    0.0
 SODIU-01         0.0    0.0    0.0    0.0    0.0
 HYDRO-01         0.0    0.0    0.0    0.0    0.0
 H3O+         1.8152-18 5.9646-08 6.2122-15 6.2188-15 1.5041-19
 NA+           3.6156   0.0    5.4259   5.4259   0.2996
 NAOH(S)         1.8103   0.0    0.0    0.0    0.1500
 NAOH:(S)         0.0    0.0    0.0    0.0    0.0
 NACL(S)          0.0    0.0    0.0    0.0    0.0
```

```
 CL-          0.0    0.0    0.0    0.0    0.0
 OH-          3.6156 5.9646-08   5.4259   5.4259   0.2996
 1-HEX-01        0.0    0.0    0.0    0.0    0.0
TOTAL FLOW:
 KMOL/HR        21.0883  33.0338  55.9324  55.9324   1.7475
 KG/HR        434.0470  595.1129 1029.1600 1029.1600  35.9675
 L/MIN         4.7888   9.9467  14.1129  14.1128   0.3968
STATE VARIABLES:
 TEMP  C       25.0000  25.0000  54.4514  54.4631  25.0000
 PRES  BAR       1.0133   1.0133   1.0133   1.2133   1.0133
 VFRAC         0.0    0.0    0.0    0.0    0.0
 LFRAC         0.9142   1.0000   1.0000   1.0000   0.9142
 SFRAC        8.5845-02   0.0    0.0    0.0   8.5845-02
ENTHALPY:
 CAL/MOL      -6.6600+04 -6.8311+04 -6.5455+04 -6.5455+04 -6.6600+04
 CAL/GM       -3235.7797 -3791.8538 -3557.3302 -3557.3169 -3235.7797
 CAL/SEC      -3.9013+05 -6.2683+05 -1.0170+06 -1.0170+06 -3.2329+04
ENTROPY:
 CAL/MOL-K      -32.5046  -38.9708  -33.8913  -33.8908  -32.5046
 CAL/GM-K       -1.5792  -2.1632  -1.8419  -1.8419  -1.5792
DENSITY:
 MOL/CC       7.3394-02 5.5351-02 6.6054-02 6.6054-02 7.3394-02
 GM/CC         1.5106   0.9972   1.2154   1.2154   1.5106
AVG MW         20.5824  18.0153  18.4001  18.4001  20.5824

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                STREAM SECTION

OFFA OFFA-P OMEGA-3 PRODUCT WASTEH2O
------------------------------------

STREAM ID        OFFA    OFFA-P   OMEGA-3  PRODUCT  WASTEH2O
FROM :         BASEREAC  P-DIST   DECANT   ACIDREAC  WASTE
TO  :         P-DIST   DIST    ----    DECANT   ----

SUBSTREAM: MIXED
PHASE:         LIQUID   LIQUID   LIQUID   LIQUID   LIQUID
COMPONENTS: KMOL/HR
 WATER         45.2168  45.2168   0.0    82.0273  83.9248
 METHA-01       31.6513  31.6513   0.0    0.1583   0.1583
 EPAME         0.0    0.0    0.0    0.0    0.0
 DHAME         0.0    0.0    0.0    0.0    0.0
 OEPA          4.2543   4.2543   0.0    0.0    0.0
 ODHA          0.2673   0.2673   0.0    0.0    0.0
 EPA          0.0    0.0    4.2543   4.2543   0.0
 DHA          0.0    0.0    0.2673   0.2673   0.0
 SODIU-01        0.0    0.0    0.0    0.0    0.0
 HYDRO-01        0.0    0.0    0.0   4.8851-14 6.5296-21
 H3O+        2.3987-15 2.4135-15   0.0    0.4496 1.3623-07
 NA+          5.4259   5.4259   0.0    5.4259   5.8756
 NAOH(S)         0.0    0.0    0.0    0.0    0.0
 NAOH:(S)        0.0    0.0    0.0    0.0    0.0
 NACL(S)         0.0    0.0    0.0    0.0    0.0
 CL-          0.0    0.0    0.0    5.8756   5.8756
 OH-          0.9043   0.9043   0.0   9.7029-15 1.3624-07
 1-HEX-01      3.1048-02 3.1048-02   0.0   1.2652-03 1.2652-03
TOTAL FLOW:
 KMOL/HR        87.7511  87.7511   4.5216  98.4596  95.8355
 KG/HR        3341.4985 3341.4985 1374.5535 3199.0755 1860.4895
 L/MIN         67.7794  67.7851  27.8289  54.8520  27.4033
STATE VARIABLES:
 TEMP  C       65.0000  65.1077  25.0000  25.0000  29.5886
 PRES  BAR       1.0133   1.8000   1.2000   1.2000   1.0133
 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:
 CAL/MOL      -6.2423+04 -6.2420+04 -6.5357+04 -6.5898+04 -6.5833+04
 CAL/GM       -1639.2983 -1639.2210 -214.9927 -2028.1636 -3391.1324
 CAL/SEC      -1.5216+06 -1.5215+06 -8.2089+04 -1.8023+06 -1.7525+06
ENTROPY:
```

```
 CAL/MOL-K       -53.3800  -53.3724 -186.9443  -41.8978  -34.7427
 CAL/GM-K        -1.4018   -1.4016  -0.6150   -1.2895   -1.7896
DENSITY:
 MOL/CC        2.1578-02 2.1576-02 2.7080-03 2.9917-02 5.8287-02
 GM/CC          0.8217    0.8216    0.8232    0.9720    1.1315
AVG MW          38.0793   38.0793   303.9965   32.4913   19.4134
```


PHYSICAL PROPERTY TABLES SECTION

PROPERTIES TABLE: PURE-1

SINGLE-PHASE PROPERTIES FOR THE MIXTURE: (KMOL/HR   )
OEPA   1.000   , ODHA   1.000   ,

VARIED VARIABLE(S): TEMP   PRES

PROPERTY SET(S): $PS-PURE

PROPERTY OPTION SET: ELECNRTL ELECTROLYTE NRTL / REDLICH-KWONG
HENRY-COMPS ID: GLOBAL
CHEMISTRY ID: GLOBAL - TRUE SPECIES

PHYSICAL PROPERTY TABLES SECTION

PROPERTIES TABLE: PURE-1 (CONTINUED)

TEMP	PRES	PL LIQUID OEPA	PL LIQUID ODHA
C	BAR	PSIA	PSIA
0.0	1.0133	3.0605-11	4.3006-12
2.0000	1.0133	4.1007-11	5.8358-12
4.0000	1.0133	5.4712-11	7.8842-12
6.0000	1.0133	7.2698-11	1.0606-11
8.0000	1.0133	9.6207-11	1.4207-11
10.0000	1.0133	1.2681-10	1.8953-11
12.0000	1.0133	1.6651-10	2.5181-11
14.0000	1.0133	2.1781-10	3.3324-11
16.0000	1.0133	2.8386-10	4.3930-11
18.0000	1.0133	3.6858-10	5.7693-11
20.0000	1.0133	4.7690-10	7.5485-11
22.0000	1.0133	6.1490-10	9.8406-11
24.0000	1.0133	7.9011-10	1.2783-10
26.0000	1.0133	1.0119-09	1.6547-10
28.0000	1.0133	1.2916-09	2.1346-10
30.0000	1.0133	1.6434-09	2.7445-10
32.0000	1.0133	2.0844-09	3.5170-10
34.0000	1.0133	2.6355-09	4.4924-10
36.0000	1.0133	3.3223-09	5.7202-10
38.0000	1.0133	4.1756-09	7.2609-10
40.0000	1.0133	5.2327-09	9.1887-10
42.0000	1.0133	6.5387-09	1.1594-09
44.0000	1.0133	8.1478-09	1.4585-09
46.0000	1.0133	1.0125-08	1.8295-09
48.0000	1.0133	1.2548-08	2.2885-09
50.0000	1.0133	1.5509-08	2.8547-09
52.0000	1.0133	1.9120-08	3.5514-09
54.0000	1.0133	2.3510-08	4.4062-09

```
!  56.0000 !   1.0133 ! 2.8836-08 ! 5.4525-09 !
!  58.0000 !   1.0133 ! 3.5282-08 ! 6.7299-09 !
!-----------+-----------+-----------+-----------!
!  60.0000 !   1.0133 ! 4.3065-08 ! 8.2856-09 !
!  62.0000 !   1.0133 ! 5.2439-08 ! 1.0176-08 !
!  64.0000 !   1.0133 ! 6.3704-08 ! 1.2466-08 !
!  66.0000 !   1.0133 ! 7.7212-08 ! 1.5236-08 !
!  68.0000 !   1.0133 ! 9.3374-08 ! 1.8578-08 !
-----------------------------------------------------
```


PHYSICAL PROPERTY TABLES SECTION

PROPERTIES TABLE: PURE-1 (CONTINUED)

```
-----------------------------------------------------
! TEMP   ! PRES   ! PL     ! PL     !
!      !      ! LIQUID  ! LIQUID  !
!      !      ! OEPA   ! ODHA   !
!      !      !      !      !
! C     ! BAR    ! PSIA   ! PSIA   !
!      !      !      !      !
!============!============!============!============!
!  70.0000 !   1.0133 ! 1.1267-07 ! 2.2600-08 !
!  72.0000 !   1.0133 ! 1.3565-07 ! 2.7431-08 !
!  74.0000 !   1.0133 ! 1.6298-07 ! 3.3220-08 !
!  76.0000 !   1.0133 ! 1.9540-07 ! 4.0142-08 !
!  78.0000 !   1.0133 ! 2.3379-07 ! 4.8403-08 !
!-----------+-----------+-----------+-----------!
!  80.0000 !   1.0133 ! 2.7915-07 ! 5.8240-08 !
!  82.0000 !   1.0133 ! 3.3264-07 ! 6.9930-08 !
!  84.0000 !   1.0133 ! 3.9561-07 ! 8.3795-08 !
!  86.0000 !   1.0133 ! 4.6959-07 ! 1.0021-07 !
!  88.0000 !   1.0133 ! 5.5634-07 ! 1.1960-07 !
!-----------+-----------+-----------+-----------!
!  90.0000 !   1.0133 ! 6.5790-07 ! 1.4246-07 !
!  92.0000 !   1.0133 ! 7.7656-07 ! 1.6937-07 !
!  94.0000 !   1.0133 ! 9.1498-07 ! 2.0098-07 !
!  96.0000 !   1.0133 ! 1.0761-06 ! 2.3805-07 !
!  98.0000 !   1.0133 ! 1.2635-06 ! 2.8144-07 !
!-----------+-----------+-----------+-----------!
!  100.0000 !   1.0133 ! 1.4809-06 ! 3.3215-07 !
-----------------------------------------------------
```


PROBLEM STATUS SECTION

BLOCK STATUS

```
**************************************************************************
*                                                                        *
* Calculations were completed with warnings                              *
*                                                                        *
* The following Unit Operation blocks were                               *
* completed with warnings:                                               *
*  DIST   BASEREAC P-DIST                                                *
*                                                                        *
* All streams were flashed normally                                      *
*                                                                        *
* All Sensitivity blocks were completed normally                         *
*                                                                        *
* All Property Tables were completed normally                            *
*                                                                        *
* Properties estimation was completed normally                           *
*                                                                        *
**************************************************************************
```