University of Pennsylvania

Senior Design

Production of Acrylic Acid from Ethylene

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Mr. Leonard Fabiano
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Dear Mr. Fabiano,

Enclosed is our design for an ethylene based acrylic acid production plant in fulfillment of the design problem proposed by Mr. John Wismer. In this report, we investigate the potential for ethylene based acrylic acid to pose a threat to the propylene based business due to the natural gas boom in the US. The investigation involves designing the epoxidation of ethylene using microchannel technology, carbonylation of ethylene oxide to β-propiolactone using a homogeneous, cobalt catalyst, and acid catalyzed rearrangement of β-propiolactone.

The report focuses on plant design and an economic analysis to determine the threat posed in the US by recent price changes in the cost of ethylene due to shale gas. The plant is designed to operate 24 hours a day for 350 days a year, with a yearly production rate of 300M lbs of acrylic acid. Economics were calculated based on the entire plant and based on ethylene-oxide cost plus analysis. For the entire plant, total permanent investment would entail $ $560M with profitability depending closely on the total permanent investment. Using present ICIS commodity chemical pricing, the Project has an IRR of 13.48% with a NPV of -$50M after 35 years. Using cost plus analysis, the non-EO section of the plant has a total capital investment of $120M with an IRR of 42.17% and an NPV of $288M over 35 years. Details regarding the process equipment and plant profitability are enclosed, along with safety requirements.

Based on this analysis, further design work must be taken verify the assumptions that have been made for this process. Determining the price and effectiveness of the microchannel reactor is key for evaluating the benefits of using a process that is void of inerts and diluents. It is crucial that pilot plant work should be undertaken to understand the true kinetics behind the carbonylation of β-propiolactone since the kinetics determine the necessary resonance time, the reactor size, per pass conversion, and overall efficiency. Pilot plant testing should be undertaken to determine the ratio of β-propiolactone to phosphoric acid needed for rearrangement on a larger scale. Reconciling this information with the data in this project would paint a clearer picture to the profitability of ethylene-based acrylic acid using cost-plus analysis. At this stage, the group concludes the idea that ethylene based acrylic acid could be a threat to propylene based manufacturers cannot be disqualified and should be further investigated.

Sincerely,

Rahul Puranmalka Minsk Jun Patricia Campos

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Section 1 – Abstract

A preliminary process design and economic analysis into the possible threat of ethylene-based acrylic acid manufacture is presented. Pipeline ethylene is fed at 14,000 ft^2/hr to the first block of this process. The epoxidation of ethylene to ethylene oxide takes advantage of microchannel technology and eliminates the need for inerts, thus decreasing equipment sizing downstream while achieving a yield of 80% overall. The resulting ethylene oxide stream is carbonylated in a liquid phase, homogeneous reaction. The β-propiolactone is then rearranged in phosphoric acid to produce 37,000 lbs of acrylic acid per hour for a yearly rate of just over 300M pounds at greater than 99.4% mass purity. The product contains 300 ppm mono-methyl ether hydroquinone to prevent the product from polymerizing and entering the explosive limits.

Using an after tax discount rate of 15%, the NPV is -$50M in December, 2014, 35 years from construction start date. The IRR is 13.84% and confirms the notion that a microchannel costs need to be further evaluated to determine the profitability. In the project, the EO plant accounts for 90% of the equipment cost and 50% of the total invested capital cost.

A cost plus analysis of ethylene oxide costs was determined and IRR data was determined based on the variability of ethylene prices and the cost-plus price of producing ethylene oxide. It was determined that the project has an IRR of 42.17% with a NPV of $288M when an after tax cash flow analysis was conducted with an after tax discount rate of 15%.

It was concluded that the feasibility of this project depends heavily on the cost of the microchannel reactors, and at this stage, the costs of the microchannel do not outweigh the advantages offered by the new reactor. It is recommended that further analysis be done to more accurately cost the microchannel reactor and to investigate the benefits of increasing the per pass conversion of ethylene. Further analysis on the reactor designs and rates for the carbonylation step and rearrangement step could help hone in the reality of an ethylene based acrylic acid process. Most importantly, further economics should be conducted to see if the best-case scenario assumptions used in this paper are too ideal. The new economics should be compared to the sensitivity analysis conducted in this study.

Section 2 – Introduction

2.1 Product

Acrylic acid is the simplest unsaturated carboxylic acid and is a building block for thousands of consumer products. It is a commodity chemical with a current market demand of nearly 10 billion pounds per year, projected to surpass 13 billion pounds worth $14 billion by the end of 2018. Acrylic acid plays an integral role in and is the monomer for polymerization used for super absorbent polymers (SAPs). Increasing population, increasing lifespan, and improving lifestyle have all significantly increased the demand and growth of super absorbent polymers market in the developed and developing world which includes disposable hygiene products such as baby diapers, and sanitary napkins. The majority of the market growth is projected to occur in China and India as these countries produce increasing amounts of products using acrylic acid as intermediates with application including detergents, coatings, adhesives, sealants, as well as personal care items. Currently, the US accounts for 25% of global production.

The product is able to undergo many reactions due to its pair of conjugated double bonds. The ability of the carbon – carbon double bond to undergo free radical reactions leads to its vast utility in polymerization reactions while the carboxyl group allows for nucleophilic displacement reactions as well as esterification reactions. These joint functionalities constitute convenient pathways to complicated heterocyclic materials. Due to the reactivity of the vinylic carbon – carbon double bond, inhibitors must be added to the product to prevent unwanted polymerizations.

Generally, acrylic acid is produced using propylene. Propylene is a byproduct of hydrocarbon cracking and naphtha refining, and the price very closely follows that of oil. Because of high refinery production rates in the US, propylene has been sold at a slight discount to ethylene historically. However, the US has seen a recent shale gas boom that has increased the supply of natural gas and ethane and dropped their prices to the lowest ever seen. With the announcement of large scale ethane crackers such as the $6 billion cracker ConocoPhillips plants to have operational by 2017, the price and supply of ethylene may soon flood US markets. The purpose of this report was to determine whether ethylene based processes could underscore and outcompete the propylene based business.

2.2 Current Methods of Production

The earliest synthesis of acrylic acid occurred in 1843 via the oxidation of acrolein. Since 1927, the commodity chemical has been commercially available through many different production means, including the Ethylene cyanohydrins process, the Reppe Process, the β-Propiolactone Process, and the Acrylonitrile hydrolysis. There is also ongoing research on microbe development to produce 3 – hydroxypropionic acid by fermentation, followed by a dehydration reaction to form acrylic acid.

The most common process for production of acrylic acid is the two stage oxidation of propylene. This process employs highly active and very selective heterogeneous catalysts consisting of metal oxides such as vanadium and molybdenum to oxidize propylene to acrolein in the first step. Yields of greater than 85% are possible.

$$C_3H_6 + O_2 \rightarrow C_3H_4O \quad (2.1)$$
$$C_3H_4O + O_2 \rightarrow C_3H_4O_2 \quad (2.2)$$

The second step involves the further oxidation of acrolein to acrylic acid using cobalt-molybdenum oxides at reactions temperatures of 200 to 300^{o}C with contact times of around 2 seconds. This current process gives acrylic acid yields of around 80-90% after absorption by water.

2.3 Proposed Production Method

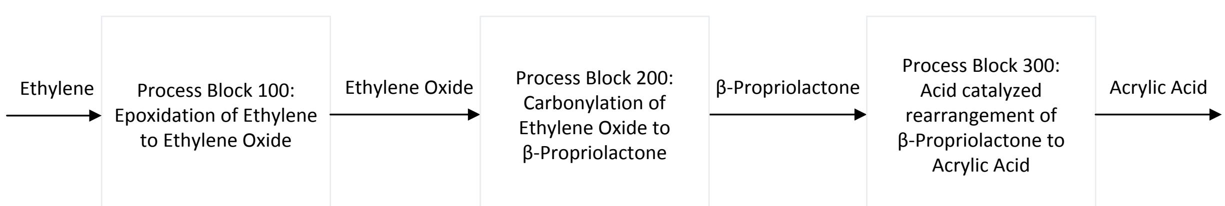


Figure 2.1

This design project investigates an ethylene based production platform. Ethylene will be oxidized to its epoxide, which will then be carbonylated to β–propiolactone. The propiolactone intermediate will then be treated with a concentrated phosphoric acid to allow for rearrangement to acrylic acid. The project is envisioned as three main reaction steps including ethylene oxidation, carbonylation of ethylene oxide, and acid catalyzed rearrangement of β-propiolactone (Allen et al, 2012).

2.3.1 Step 1: Oxidation of Ethylene

$C_2H_4 + O_2 \rightarrow C_2H_4O$

Figure 2.1

The most common method for making EO entails a vapor-phase, direct oxidation of ethylene with high purity oxygen in a tubular reactor. The process utilizes silver catalyst on α-alumina support in the form of rings or lobed shapes to increase the surface area. Trace amounts of other elements such as Cs and Re are added to the catalyst to increase selectivity to EO. The reaction occurs in the presence of recycled CO_2 and inert gases including methane, nitrogen, and argon, inerts deliberately included to bring ethylene and oxygen out of the flammability region and terminate free-radicals, thus preventing a runaway reaction. Inerts also help the reaction conditions by increasing heat capacity of the stream and improving heat removal from the exothermic reaction, helping to maintain a smaller temperature profile. Trace amounts of chlorinated compounds are added continuously to the reactor feed to inhibit the undesired combustion of ethylene.

The epoxidation of ethylene generally operates at a selectivity of 80-90% based on the industrial grade silver α-alumina catalyst used. Increasing the temperature increases the reaction rate, but decreases the selectivity, Thus, in an effort to maximize selectivity, the per pass ethylene conversion is kept between 10-20% and the reactor temperature is generally maintained around 240-290°C and 15-25 bar. Heat removal is important to maintain selectivity and prevent hotspots from occurring. Reactors are generally oil or boiling water cooled to maintain a temperature within the acceptable operating range.

EO is recovered from the reactor product by absorption in process water to prevent the retention of other gases and light components. It is then stripped from the water, which includes removing water and trace amount of formaldehyde and acetaldehyde. EO is then sent to a purification section where the water and EO mix are separated, resulting in an EO stream around 99.5% purity.

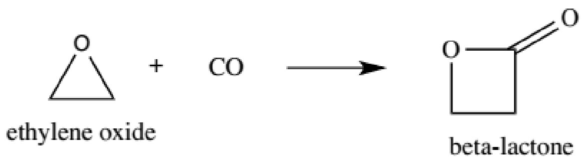
The rest of the components need to be recycled due to the low per pas conversion of ethylene (around 10-20%) to prevent the waste of ethylene. CO_2 needs to be removed to prevent buildup in the system and minimize the purge loss. The presence of other gases with similar molecular weight and polarity such as methane, formaldehyde, and argon makes this separation difficult. Thus, the unreacted ethylene and oxygen, by-product CO_2, and inert gases not absorbed are then sent to a CO_2scrubbing unit that typically uses MEA to scrub the gas or employs the Benfield Process, owned by UOP, which uses K_2CO_3 as a reagent to react with the CO_2 to produce $HKCO_3$. The $HKCO_3$ is then decomposed to CO_2 which is then disposed of.

Older versions of EO plants use air, but most air-based plants have been converted to cryogenic oxygen. This generally increases the selectivity and decreases the amount of nitrogen in the system, thus reducing the size of equipment and permitting a more concentrated reactor inlet feed which increases the selectivity to EO. These advantages generally outweigh the costs of providing and handling pure oxygen.

This project proposes the use of a microchannel reactor for the oxidation reaction. Microchannel reactors offers many advantages over a tubular reactor. In a tubular reactor, the massive amount of heat can cause hot spots and heat removal problems which can lead to bad selectivity or runaway, considering that while epoxidation is -105 kJ/mol, total combustion is around -1250 kJ/mol. As described by *Kestenbaum, et al*, the microchannels are around 500µm by 50µm. This leads to an enhanced surface-to-volume ratio and enables effective heat management. *Steif et al* showed that microchannels could be controlled to a maximum temperature gradient of 1ºC, which would be very beneficial for selectivity. Also, relatively large ratio of surface area acts as a natural free-radical terminator, so inerts such as nitrogen and argon would not have to be added for the reaction. If an explosion where to occur, microchannel reactors are strong enough to withstand it and continue operation.

In theory, the use of a microchannel reactor system would allow for the process to occur without inerts or to allow for operation in the flammable region. Although microchannel reactors are not presently used in commercial EO production, we chose this method in order to obtain the most favorable economics for the ethylene-based process. In order to minimize reactor volumes, pure oxygen is utilized throughout the process.

2.3.2 Step 2: Carbonylation of Ethylene Oxide



$C_2H_4O + CO \rightarrow C_3H_4O_2$

Figure 2.2

The ethylene oxide product from the first step is combined with carbon monoxide obtained from the gulf coast in the second step to produce β-propiolactone. Due to its toxicity, the propiolactone will not be isolated. This is a liquid phase, catalyzed reaction with pressure maintained through the use of CO.

The catalyst used is $[Co(CO)_4][TPP]$ and the amount of catalyst was determined from the literature to be 15 mM. Church et al. (2006) have shown that the rate does not vary with the amount of propylene oxide or CO but does vary linearly with the amount of catalyst. Since the structure of propylene oxide is very similar to that of ethylene oxide, a technical assumption was made that the order of kinetics would be similar. However, it should be noted that with a more complex form of epoxide, such as 4,5-octane oxide, have reported first order carbonylation kinetics (Mulzer et al, 2014, Rowley, 2007). Although Allen et al. (2012) have presented some data for absorbance of ethylene oxide, acetaldehyde, and β-propiolactone, the lack of clarification of how the absorbance varies with the concentration did not allow us to make conclusions about the kinetics.

Another technical assumption relates to the stability of the catalyst at higher temperatures. As the patent results have shown, the catalyst maintains its stability and does not decompose at 80 °C. The promoter TPP has a boiling point of over 300 °C, and it bonds to metal carbonyl complexes. Therefore, it was assumed to be stable under high temperatures such as 240 °C.

Production of β-propiolactone from ethylene oxide is a relatively new process, and to our knowledge there are no plants whose operations involve using this reaction. As propylene is the traditional precursor to acrylic acid production, and production from propylene involves only oxidation steps, few similarities are found in this process and the traditional process as propylene as cursor.

However, as this reaction is a carbonylation process, it bears many similarities with other processes such as the production of acetic acid. The Monsanto process is a metal carbonyl catalyst-catalyzed reaction that produces acetic acid from methanol, was later improved upon by BP. A typical acetic acid plant that employs the Monsanto process has a single reactor followed by a series of distillation columns to purify the acetic acid, and the solvent, catalyst, and unused reactants are recycled back into the reactor (Asaoka et al, 1994, Souma, 1991). This process usually takes place under 150-200 C and 30 bar and has high acetic acid selectivity (Van Leeuwen and Claver, 2001).

There are key differences between the acetic acid process and the production of β-propiolactone. The former is first order, while the latter is assumed to be zeroth order. The operating temperature of β-propiolactone production is much lower, while the pressure is similar. Because the reaction is zeroth order, a large amount of production per year may necessitate parallel CSTRs.

A total of 677.57 lb/hr of sulfolane and 2.173 lb/hr of catalyst are recharged into the system to replace the purged sulfolane in the stoichiometric amount. This purged stream will contain, in addition to sulfolane, undistilled β-propiolactone and other side products such as succinic anhydride. Many of these side products, especially high-boiling compounds like succinic anhydride, are difficult to remove fully from sulfolane (Fumagalli, 2001). Because purchasing the replacement sulfolane and catalyst will be expensive, the purged sulfolane can undergo batch distillation in regular intervals to remove impurities and only leave sulfolane and catalyst. As the sulfolane will need to be heated to high temperatures, the assumption that the catalyst will be stable at high temperatures above 350 C must be tested in the laboratory.

2.3.3 Step 3: Acid-Catalyzed Rearrangement of β-Propiolactone

$C_3H_4O_2 \rightarrow C_3H_4O_2$

Figure 2.3

Phosphoric acid and propiolactone are mixed in the third step to induce a homogenously acid catalyzed rearrangement yielding the acrylic acid product. The reaction is carried out in the liquid phase under vacuum at high temperature. The reactor is initially charged with the requisite amount of phosphoric acid catalyst. The catalyst is maintained in the liquid phase by adding trace amounts of water when the viscosity of the acid increases significantly. As the reaction proceeds, acrylic acid vapors are produced at relatively the same rate as the β-propiolactone feed rate. At this point, mono methyl ether hydroquinone (MEHQ) is added as an inhibitor to prevent the polymerization of the acrylic acid product.

In a similar process, which is no longer used, ketene is first reacted with formaldehyde in the presence of a Freidel Crafts catalyst, such as aluminum tricholoride, to form β-propiolactone. The lactone is then treated in a process similarly to that described above, with the exception of the MEHQ inhibitor. In this case a copper inhibitor was used. This process was popularized by Celanese during the years 1957 to 1974 and produced 35,000 tonnes of acrylic acid per plant (Arpe 2010).

Assumptions were made regarding the amount of phosphoric acid catalyst required in the final rearrangement step. As discussed by Schnizer and Wheeler, Phosphoric acid was supplied at a rate so that at least ten percent of the β propiolactone feed rate was present at all times inside of the reactor. This process uses a per pass conversion based on β-propiolactone of 0.97 with an overall conversion of 0.995. Again as discussed by Schnizer and Wheeler, the production rate of any side products were assumed to be negligible. Reaction kinetics were considered to be first order in lactone, as is typical with most other acid catalyzed reactions. The feed rate of β-propiolactone listed in patent 3,176,042 was 0.116 grams per gram H_3PO_4 per hour. This amount of phosphoric acid requires a reactor volume of 54,000 gallons. Because the example listed in the patent was performed at the bench scale, it was suggested a feed rate of 0.9 gram per gram H_3PO_4 per hour for our scaled up process, provided adequate mixing (personal correspondence).

2.4 Customer Requirements

Acrylic acid is a commodity chemical with a market demand of nearly 10 billion pounds per year. About 65% of production is used as a platform for ester synthesis while the other 35% is purified to glacial acetic acid.

Acrylic acid is generally produced in two grades including the crude or technical grade which has a mass purity of about 94%. Maleic anhydride, propionic acid, and acetic acid constitute the main impurities. This grade is suitable starting material for a variety of acrylic esters used in producing surface coatings, adhesives and sealants, and other plastics. The glacial grade refers to acrylic acid with purities of greater than 98% and is typically used for the production of super absorbent polymers.

2.5 Commercial Applications

The main use of acrylic acid is as feedstock for the production of commodity chemicals, notably acrylate esters. The esters are responsible for many desirable features in polymers such as acid and base resistance, optical properties, in addition to heat and aging resistance. Notable esters include the methyl ester of acrylic acid which is used as a copolymer component of acrylic acid fibers. The ethyl ester finds applications in the fabrication of paints, both water and solvent based, while the butyl ester is used mainly in adhesives. Acrylic acid polymerizes easily to give polyacrylic acid. This polymer is important for coatings, paints, adhesives, and other textiles.

2.6 Project Charter

Project Name	Acrylic Acid from Ethylene
Project Champions	Mr. Leonard Fabiano, Dr. Raymond Gorte, Mr. John Wismer
Project Leaders	Patricia Campos, Minsik Jun, Rahul Puranmalka
Specific Goals	Cost effective means of production of Acrylic Acid at 300 million lbs/yr using a 3 step process with ethylene as the precursor.
Project Scope	Annual acrylic acid production of 300 million lbs/yr Ethylene pricing "Cost plus" based on quoted prices of ethane Incorporating microchannel reactors to prevent hot spots and heat removal problems in the epoxidation step Choosing a catalyst and solvent for the carbonylation step (step 2) Applying kinetic data from batch results to a continuous process (step 2) Choosing a catalyst and polymerization inhibitor for the final rearrangement step
Deliverables	Late January: Preliminary Process Flowsheets including material balances Late February: Complete process synthesis along with material and energy balances Late March: Detailed design of the process units
Time Line	Senior Design Presentation: Wednesday April 23

2.7 Innovation Map

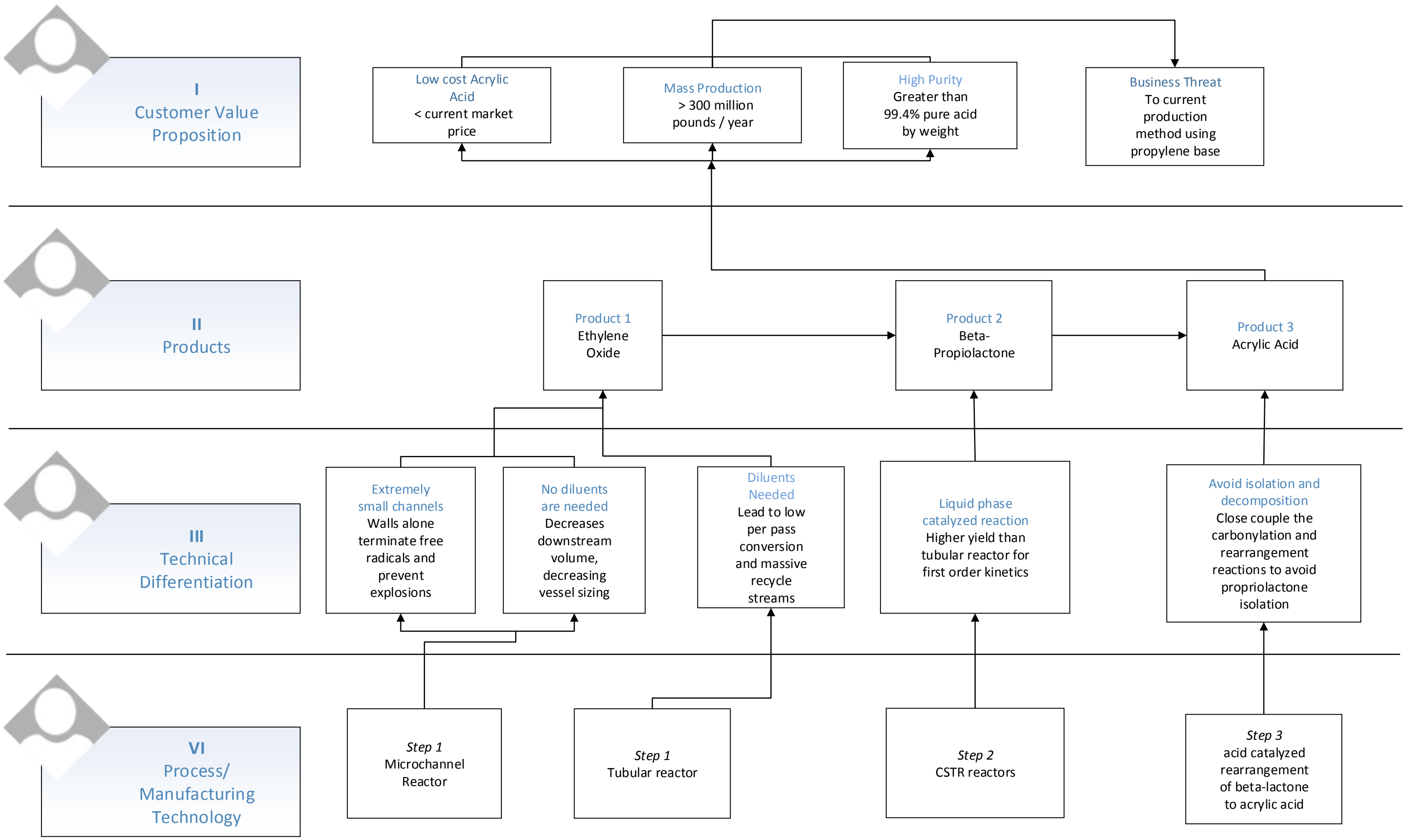


Figure 2.5

Section 3 – Process Description

3.1 Overview

In this process, best case scenario assumptions were adopted in order to address the potential ethylene based production has to be more profitable than the propylene based business. The overall process has be broken down into three blocks. Block 100 deals with the conversion of ethylene to ethylene oxide which contains four subsections; a microchannel reactor an EO gas scrubbing section, an EO purification section, and a CO_2 scrubbing section. Block 200 details the carbonylation of ethylene oxide to β-propiolactone which contains 2 subsections, CSTR reactors in series and purification. Block 300 details the phosphoric acid-catalyzed rearrangement of β-propiolactone into acrylic acid which contains 2 subsections, vacuum reactor and purification. Acrylic acid is stored in a storage tank and packaged continuously.

3.2 Block 100: Epoxidation of Ethylene to Ethylene Oxide

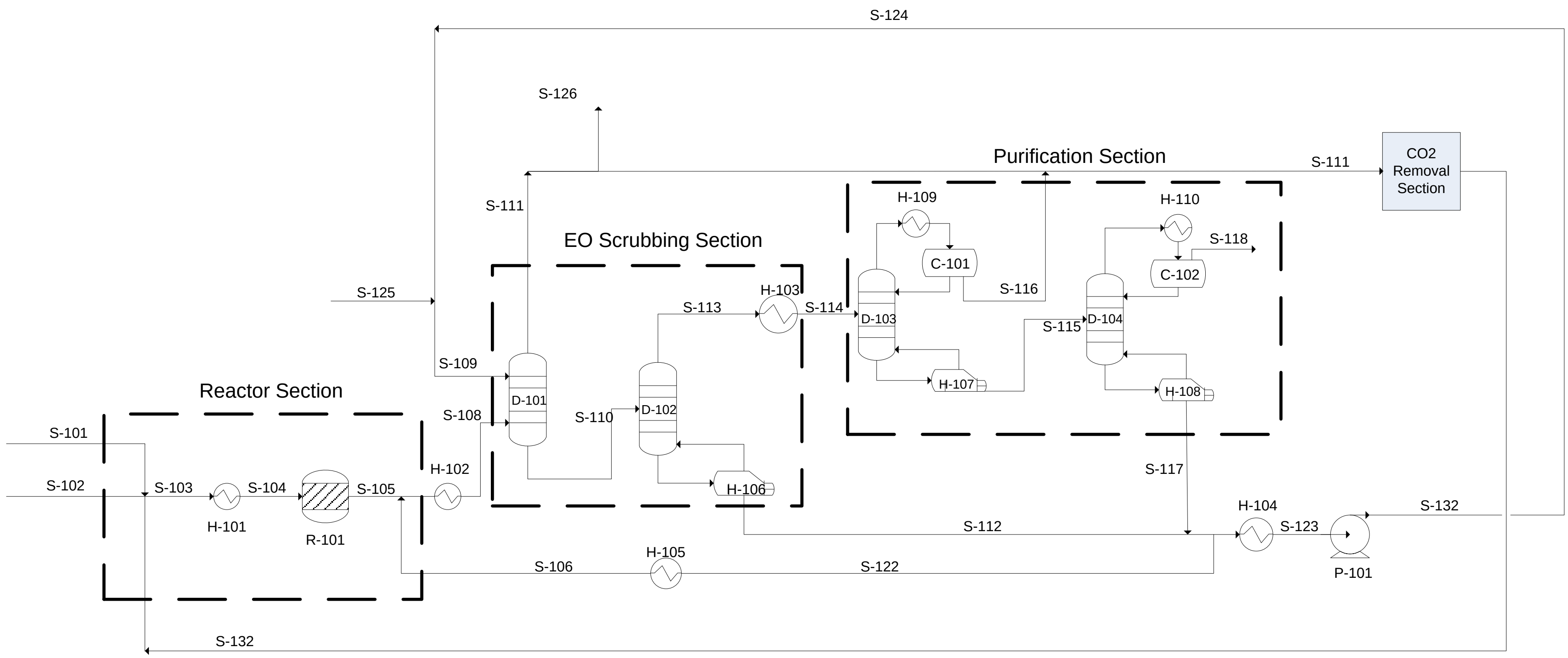


Figure 3.1

It was assumed that ethylene and oxygen will be obtained via pipeline in the gulf at pipeline prices. Thus, no storage will be necessary. The reaction would occur at best case scenario conditions.

3.2.1 Microchannel Reactor

The microchannel reactor is assumed to contain an industrial catalyst operating at the highest efficiencies know due to the small temperature profile in the reactor. Per pass conversion is set at 20% as reported in *Kestenbaum, et al.* The selectivity is set at 90% to mimic the starting industrial selectivity known with shell catalysts.

For this process, the microchannel would be that designed by Institut fur Mikrotechnik Mainz GmbH and used by *Kestenbaum, et al.* The microchannels have a mixing unit where the reactant gases are injected from opposite sides and mix in a diffusion path that is 1mm in length; modeling in FLUENT by *Kestenbaum, et al* showed that this length is sufficient to create a homogeneity of around 99%.

The reactor design for this process was taken directly from *Kestenbaum, et* al, specifically for the etched catalyst. Pricing was done using the exact process used by *Alaskan Natural Gas to Liquids*. Total cost for the microchannel reactor system is $30M.

After the ethylene oxide is produced, it needs to be scrubbed immediately. This is because the microchannel reactor does not contain inerts which serve to limit the explosive regime of ethylene, and more importantly, ethylene oxide. The microchannel from patent 0036106 contains a quenching apparatus with a mixer capable of mixing the outlet gas with low temperature steam. Steam is used since the EO will be scrubbed downstream with water. This is modeled by stream S-106 with mixer M-102.

3.2.2 Ethylene Oxide Scrubbing

Gaseous Ethylene Oxide is removed from the reactor product gas and sent to the scrubbing unit. Scrubbing is using water since EO is miscible. Process water at ambient temperature is used since process water is generally cheaper to purchase and recycle than any other agent. Flow rates are easily be adjusted to scrub out 99.9% of the EO. Process water enters the block in stream S-125 at a rate of 180 lbs/hr. This combines with recycled process water for a total water scrubbing rate of 144400 lbs/hr. The water enters the top of the absorber, D-101, operating at 200 psia. The scrubbed gas leaving the top in stream S-111 contains the majority of oxygen, ethylene, acetaldehyde, argon, and methane, which then goes to the CO2SCUB. The bottoms, S-110, goes to the stripper, D-102.

The stripper, D-102, removes the majority of water and small amounts of formaldehyde which are then recycled to the quenching stream and scrubber. The stripper operates at 150 psia, with the EO coming out of the top at 360ºF and the water leaving the bottoms at around 280ºF. The EO and other gases leave the top of the column through stream S-113 to be cooled and contain both liquid and vapor to prior to entering the first purification column, D-103. The water bottoms exits through stream S-112.

3.2.3 Ethylene Oxide Purification

EO purification occurs in two steps. D-103 removes any components lighter than EO, including methane, oxygen, ethylene, formaldehyde, carbon dioxide, and argon. The bottoms product is 33% EO, 66% Water, and the balance formaldehyde. The flue gas leaving through the top, S-116, is combined with the flue gas from D-101 to create the recycle gas stream containing unreacted ethylene and oxygen. This then goes to the CO_2 scrubbing unit. The bottoms, S-115, then enters the second purification column, D-104. This column separates the EO from the water, resulting in a product stream that is 99.4% rich. The bottoms leaves in stream S-117 and combines with the bottoms of D-102 to be recycled as the EO scrubbing agent and reactor product quenching steam.

3.2.4 CO_2 Separation

The majority of the byproducts created are due to the full combustion of ethylene, resulting in a reactor product stream of around 5% CO_2 by weight. Aqueous monoethanolamine (MEA) exhibits selective reactivity towards CO_2 and is used for the CO_2 scrubbing unit. Contacting an aqueous solution of MEA with a gas containing carbon dioxide, a series of reactions occur in the liquid phase, driving the CO_2 into the liquid, until equilibrium is established (*Fashami et al*):

$$CO_2 + 2\,H_2O \leftrightarrow HCO_3^- + H_3O^+ \qquad (3.1)$$

$$MEA\ +\ HCO_3^- \leftrightarrow MEACOO^- + H2O \qquad (3.2)$$

$$HCO_3^- + H_2O \leftrightarrow CO_3^{2-} + H_3O^+ \qquad (3.3)$$

$$MEAH^{+} + H_2O \leftrightarrow MEA + H_3O^{+} \tag{3.4}$$

$$2H_2O \leftrightarrow H_3O^{+} + OH^{-} \tag{3.5}$$

The model can be used and simulated in ASPEN. This report draws from the MEA system developed by *Alaskan Natural Gas to Liquids*.

CO2SRUB is modeled as a separation block that removes 70% of the CO2 from the inlet stream. The MEA-101 system in Alaskan Natural Gas to Liquids removes 80% of the CO2, but 70% was used for safety. The system cost is modeled using the Economies of Scale and the Six-Tenths Factor as described by Seider. Process description includes an "amine absorber that operates at 100ºF and atmospheric pressure to favor the CO2-MEA complex. It is built of stainless steel to resist MEA corrosion, and consists of 28 18ft towers. The use of more MEA and bigger equipment for more separation is not economically justified. The column consists of two packed beds modeled as equilibrium stages in which the syngas is contacted with a lean (3.7M) MEA solution. Because of the low operating pressure of the absorber and the high vapor pressure of MEA, there is a significant amount of MEA (over 500 ppm) leaving the absorption section with the clean syngas. This is removed in a flash vessel, and the resulting MEA recycled back to the absorber. Some MEA in the column is taken out, cooled, and re-circulated to cool the column." The CO2 scrubbed recycle stream then mixes with the inlet oxygen and ethylene streams and goes into the reactor. The costs of amine treating, preparation, reclamation, and storage away from air are included. The total installed cost of the system is $50,805,790.75.

3.3 Block 200: Carbonylation of Ethylene Oxide to β-Propiolactone

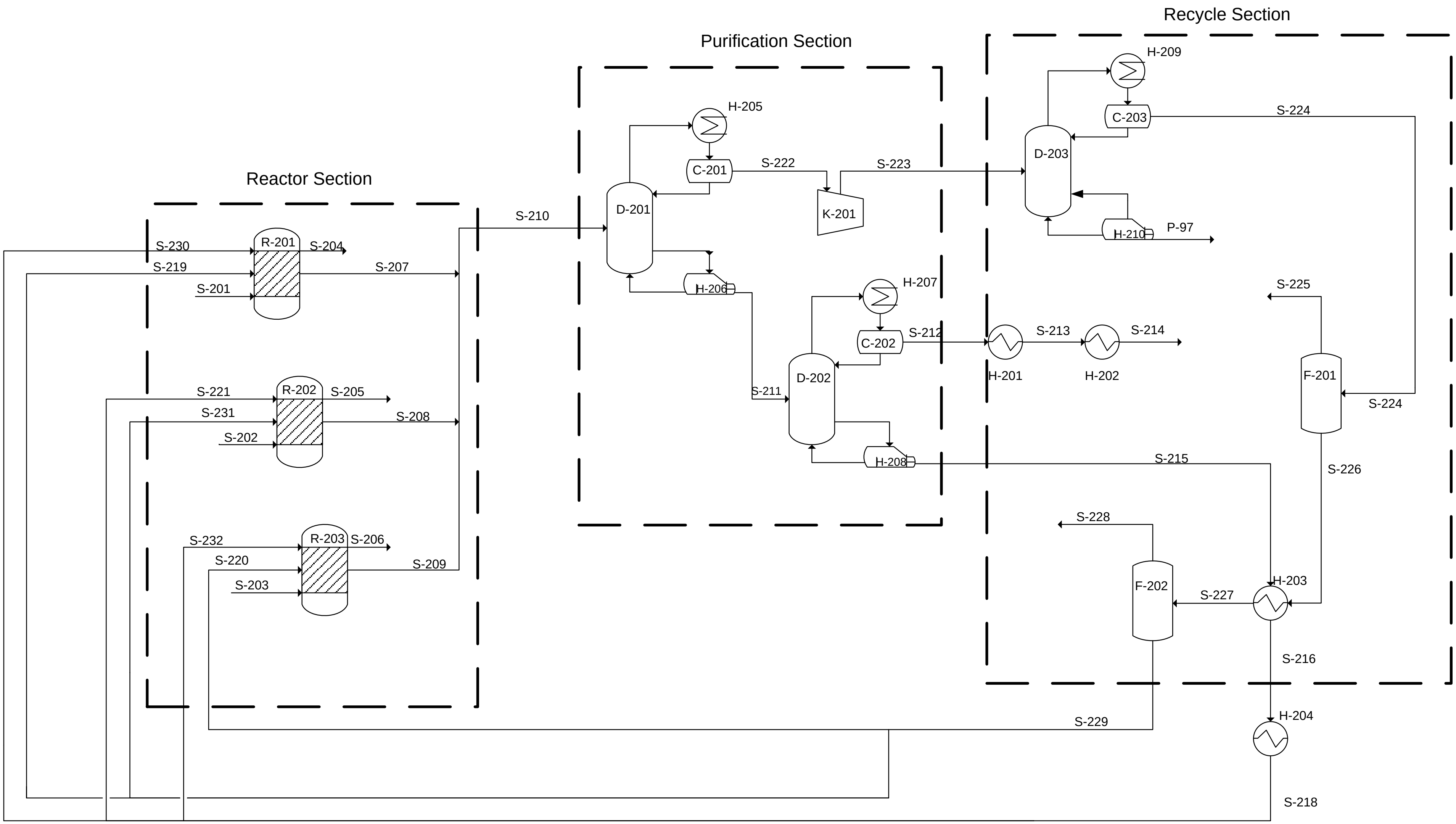


Figure 3.2

The reaction occurring here is the carbonylation of ethylene oxide to form β-propiolactone. First, selectivity percentages which showed that the reaction of initial concentration of 1.0 M ethylene oxide in sulfolane under 80 °C and 600 psi had the optimal selectivity of 95.8% and 2.8% for β-propiolactone and acetaldehyde respectively (Allen et al, 2012). For this step, a 97% overall conversion and 90% per pass conversion was assumed.

Each CSTR is sized to 8000 gallons and has a residence time of 0.198 hours in order to allow the reaction to go to completion without letting the reactors become too large. Reactors should be kept lower than 10000 gallons to allow for less power-intensive mixing.

The product streams from the CSTR's merge and enter a distillation column. This distillation column is able to easily separate the light key, acetaldehyde, from the heavy key, β-propiolactone, due to the large boiling point differences between them. The bottoms product from the first distillation column, which consists of β-propiolactone and sulfolane with the catalyst, enters another distillation column. The diameter must be substantially larger due to the higher reflux ratio in this column compared to the other ones. Due to the high reboiler temperatures needed for distillation at normal pressures, both of the distillation columns were under very low pressures to maintain the reboiler temperatures around 450 °F (232 °C). Steam injection vacuum systems were used.

Distillation column D-203 was used to minimize the amount of acetaldehyde in the recycling process of CO and ethylene oxide. Due to the small boiling point temperature difference between ethylene oxide and acetaldehyde, it was impractical to attempt to recycle all of the ethylene oxide or keep the CO-ethylene oxide stream pure; attempting to do so would have resulted in a very low condenser temperature. Instead, small amounts of ethylene oxide and most of acetaldehyde was purged through the bottoms, and large amounts of ethylene oxide and all of CO were recycled. A flash vessel is able to separate CO and ethylene oxide easily, and CO is sent to the pipeline to be fed into the CSTR's. The remaining ethylene, with a small amount of CO and acetaldehyde, is heated with a heat exchanger whose hot stream is sulfolane from D-202, and any CO and ethylene oxide that has been vaporized is purged through another flash vessel, F-202. The bottoms product from F-202 is split into three streams, each entering as a recycle into each reactor. Lactone cooler and condenser were used to reduce the pressure and temperature of the lactone. Due to the large amount of cooling required and very little heating, an extensive heat integration in this process was not possible.

3.4 Block 300: Acid Catalyzed Rearrangement of β-Propiolactone to Acrylic Acid

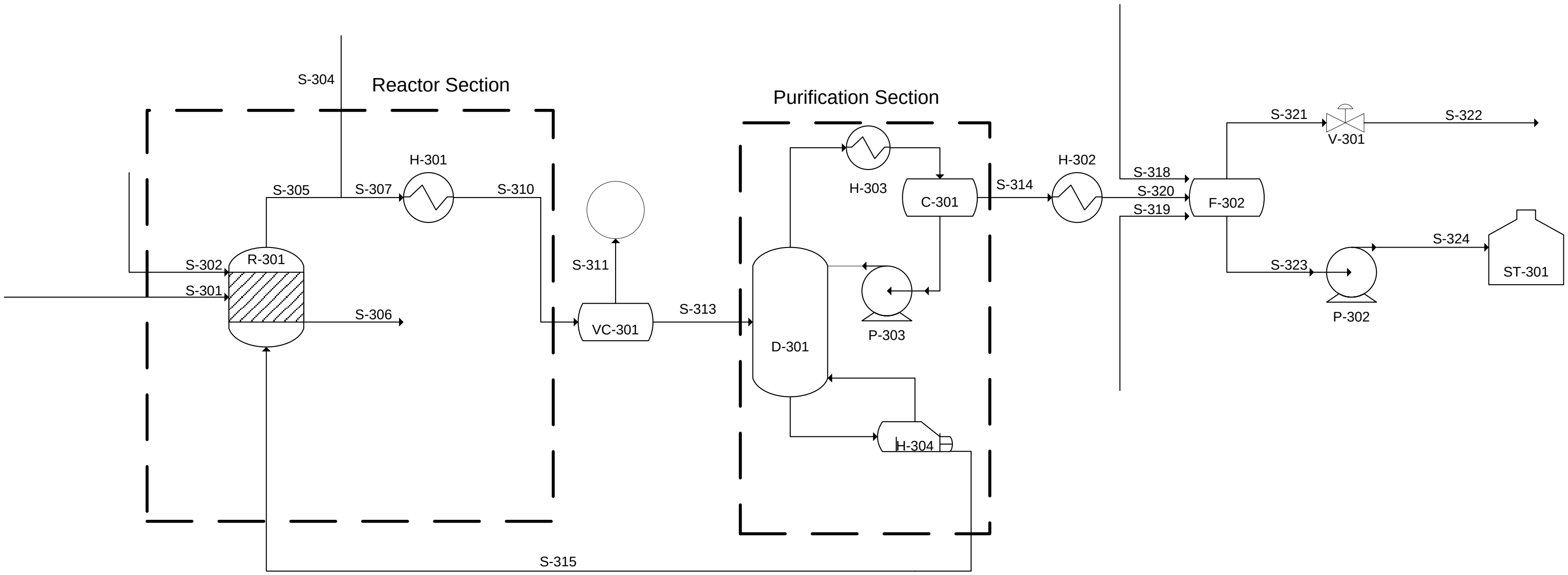


Figure 3.3

3.4.1 Reactor and Purification of Acrylic Acid

A liquid feed stream consisting of 10% mol phosphoric acid and the balance of β-lactone is fed to a stirred tank reactor. The reaction operates under vacuum at 2 psia and at a temperature of 170 degrees Celsius. The low reaction pressure allows for both operation at lower temperatures and a smaller concentration of acrylic acid product in the vessel at all times, which lowers the tendency for polymerization. The reaction temperature falls 50 degrees below the boiling point of acrylic acid at this pressure, allowing for easy removal of the vapor product. Directly following the reaction zone, MEHQ inhibitor in sprayed in the vapor product prior to condensing the acrylic acid vapors.

It is assumed throughout the process that the phosphoric acid catalyst has no vapor pressure and that no phosphoric acid will escape the reactor. The reactor will be crafted using hastelloy C, an alloy consisting of chromium, molybdenum, and tungsten, due to its chemical compatibility with phosphoric acid.

This relatively simple process is a scaled up version of a bench process. Streams S-301 and S-302, consisting of phosphoric acid and β-lactone respectively, are fed to a stirred tank reactor. The flash vessel F-301 directly following the reactor allows for the removal of acrylic acid vapors. In reality, the RStoic unit and flash vessel are envisioned as one unit with a liquid feed and vapor products. Following condensation of the acrylic acid vapors, the liquid is then pumped to 40 psia and enters distillation column D-301 on stage 7. The column is crafted of carbon steel with 16 trays and a 5.5 ft diameter. Any unreacted lactone is recycled back to the reactor (S-315). The overhead vapor product, S-314, has a 99.4% mass purity of acrylic acid with trace of amounts of β-lactone.

More MEHQ is added to the overhead product of the column to provide a concentration of around 300 ppm. A nitrogen stream is available to ensure that the flash vessel operates at atmospheric pressure. The overhead product from the flash vessel is waste nitrogen which is then sent to the flare. The bottoms product containing the acrylic acid product is then pumped to a storage vessel.

3.4.2 Acrylic Acid Storage and Handling

The vinylic functionality of acrylic acid predisposes it to unwanted polymerization reactions. Fortunately, many inhibitors exist in the literature including, phenothiazine, and hydroquinone. Hydroquinone monomethyl ether (MEHQ) was chosen for price considerations as well as its widespread use in industry. Typical concentrations of inhibitor in the product range from 50 to 500 ppm. This process uses 300 ppm for convenience.

The polymerization reaction proceeds through radical intermediates. MEHQ inhibition is much more effective in the presence of oxygen (Li and Schork, 2006). The oxygen reacts with primary radicals to form peroxy radicals which react much more slowly. The MEHQ reacts with the peroxy radicals and ultimately terminates the reaction. The MEHQ requires oxygen for the inhibition to be effective, therefore the product must be stored under air.

Acrylic acid is relatively corrosive towards most materials and must therefore be stored in glass-lined equipment, polyethylene, polypropylene, or stainless steel. Care should be taken to avoid freezing the acid as this creates non-uniformities in the concentration of the inhibitor throughout the acid. This can also create temperature gradients throughout the acid. The industrially accepted storage temperatures range from 20 to 30 degrees Celsius. While glacial acrylic acid has a freezing temperature of around 13 degrees Celsius, addition of water lowers this to around -5 degrees.

Section 4 – Flow Sheets and Stream Reports

4.1 Section 100 - Epoxidation of Ethylene

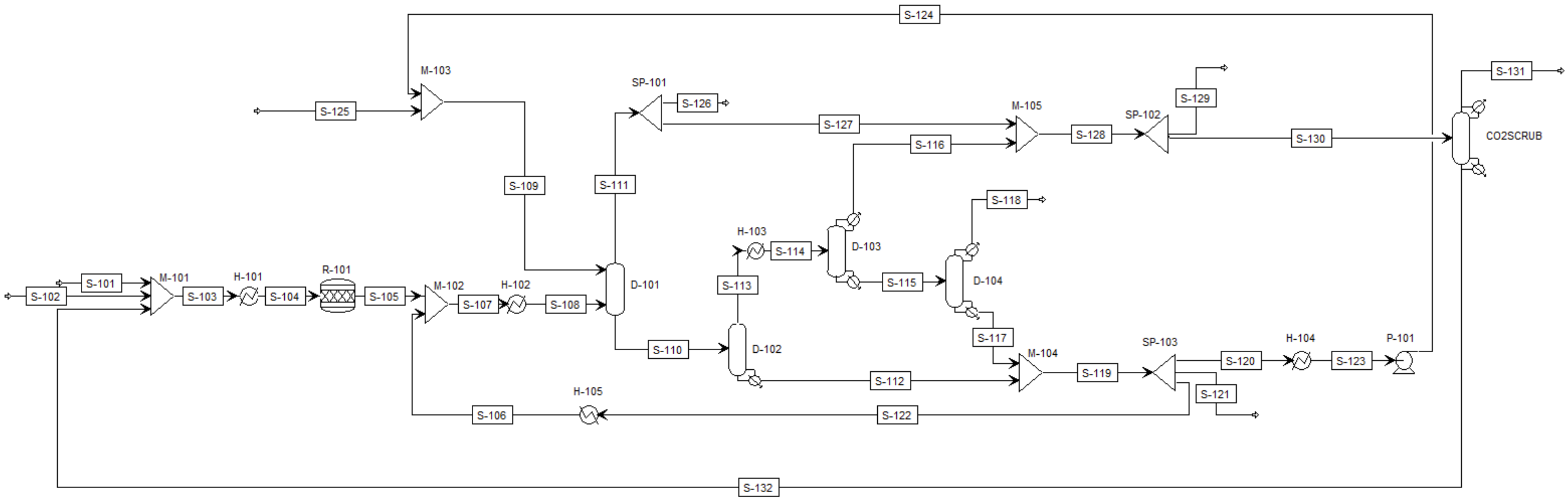


Figure 4.1

Table 4.1 Section 100 Stream Reports		S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108
		lb/hr							
Component	**Chemical Formula**								
Ethylene	C_2H_4	17,864.63	0.00	85,874.67	85,874.67	68,699.74	1.12	68,700.86	68,700.86
Oxygen	O_2	0.00	14,677.69	34,845.32	34,845.32	20,373.10	0.00	20,373.10	20,373.24
Ethylene Oxide	C_2H_4O	0.00	0.00	130.41	130.41	24,403.42	8.91	24,412.33	24,412.33
Formaldehyde	CH_2O	0.00	0.00	4,482.18	4,482.18	4,574.09	14.08	4,588.17	4,588.16
Acetaldehyde	C_2H_4O	0.00	0.00	0.04	0.04	67.46	0.05	67.51	67.51
Carbon Dioxide	CO_2	0.00	0.00	2,162.65	2,162.65	7,281.90	0.06	7,281.96	7,281.96
Water	H_2O	0.00	0.00	82.97	82.97	2,178.52	18,002.43	20,180.95	20,180.94
Argon	Ar	0.00	92.08	9,123.27	9,123.27	9,123.27	0.00	9,123.27	9,123.27
Methane	CH_4	51.34	0.00	5,089.89	5,089.89	5,089.89	0.00	5,089.89	5,089.89
Total Flow (lb/hr)		17,915.97	14,769.77	141,791.00	141,791.00	141,791.00	18,026.64	159,818.00	159,818.00
Temperature (F)		152.60	152.60	71.41	482.00	482.00	414.69	473.94	94.02
Pressure (psia)		300.00	300.00	140.00	300.00	290.08	291.00	290.08	215.00
Vapor Frac		1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.70
Enthalpy (Btu/lb)		825.71	16.58	288.71	443.68	30.38	-5,611.66	-606.01	-902.53

Table 4.2 Section 100 Stream Reports		S-109	S-110	S-111	S-112	S-113	S-114	S-115	S-116
		lb/hr							
Component	**Chemical Formula**								
Ethylene	C_2H_4	8.99	42,765.99	25,943.86	10.25	42,755.74	42,755.74	0.00	42,755.74
Oxygen	O_2	0.00	1,417.66	18,955.59	0.00	1,417.66	1,417.66	0.00	1,417.66
Ethylene Oxide	C_2H_4O	71.24	24,473.92	9.65	56.93	24,416.99	24,416.99	24,294.91	122.08
Formaldehyde	CH_2O	112.61	4,692.12	8.65	127.67	4,564.45	4,564.45	45.64	4,518.81
Acetaldehyde	C_2H_4O	0.41	67.88	0.03	0.01	67.87	67.87	67.87	0.00
Carbon Dioxide	CO_2	0.45	4,657.76	2,624.65	0.51	4,657.25	4,657.25	0.00	4,657.25
Water	H_2O	144,110.00	164,207.00	83.81	144,016.00	20,191.06	20,191.06	20,191.06	0.00
Argon	Ar	0.00	612.00	8,511.27	0.00	612.00	612.00	0.00	612.00
Methane	CH_4	0.01	719.01	4,370.88	0.01	719.00	719.00	0.00	719.00
Total Flow (lb/hr)		144,303.00	243,613.00	60,508.38	144,211.00	99,402.03	99,402.03	44,599.49	54,802.54
Temperature (F)		91.46	110.39	91.83	357.87	279.64	-28.64	191.55	3.59
Pressure (psia)		334.00	200.90	200.00	150.30	150.00	145.00	142.90	140.00
Vapor Frac		0.00	0.00	1.00	0.00	1.00	0.05	0.00	1.00
Enthalpy (Btu/lb)		-6,799.10	-4,626.96	30.01	-6,500.73	-1,162.84	-1,643.16	-3,402.47	86.19

Table 4.3 Section 100 Stream Reports		**S-117**	**S-118**	**S-119**	**S-120**	**S-121**	**S-122**	**S-123**	**S-124**
		lb/hr							
Component	**Chemical Formula**								
Ethylene	C_2H_4	0.00	0.00	10.25	8.99	0.14	1.12	8.99	8.99
Oxygen	O_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene Oxide	C_2H_4O	24.30	24,270.61	81.23	71.24	1.08	8.91	71.24	71.24
Formaldehyde	CH_2O	0.72	44.92	128.39	112.61	1.70	14.08	112.61	112.61
Acetaldehyde	C_2H_4O	0.45	67.42	0.46	0.41	0.01	0.05	0.41	0.41
Carbon Dioxide	CO_2	0.00	0.00	0.51	0.45	0.01	0.06	0.45	0.45
Water	H_2O	20,180.97	10.10	164,197.00	144,019.00	2,174.69	18,002.43	144,019.00	144,019.00
Argon	Ar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methane	CH_4	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.01
Total Flow (lb/hr)		20,206.44	24,393.05	164,417.00	144,213.00	2,177.61	18,026.64	144,213.00	144,213.00
Temperature (F)		231.74	65.14	233.15	233.15	233.15	233.15	90.00	91.46
Pressure (psia)		22.1	20	22.1	22.1	22.1	22.1	15	334
Vapor Frac		0.00	1.00	0.14	0.14	0.14	0.14	0.00	0.00
Enthalpy (Btu/lb)		-6,652.26	-524.76	-6,519.36	-6,519.36	-6,519.36	-6,519.36	-6,800.55	-6,799.10

Table 4.4 Section 100 Stream Reports		**S-125**	**S-126**	**S-127**	**S-128**	**S-129**	**S-130**	**S-131**	**S-132**
		lb/hr							
Component	**Chemical Formula**								
Ethylene	C_2H_4	0.00	2.59	25,941.27	68,697.01	686.97	68,010.04	0.00	68,010.04
Oxygen	O_2	0.00	1.90	18,953.69	20,371.35	203.71	20,167.63	0.00	20,167.63
Ethylene Oxide	C_2H_4O	0.00	0.00	9.65	131.73	1.32	130.41	0.00	130.41
Formaldehyde	CH_2O	0.00	0.00	8.64	4,527.45	45.27	4,482.18	0.00	4,482.18
Acetaldehyde	C_2H_4O	0.00	0.00	0.03	0.04	0.00	0.04	0.00	0.04
Carbon Dioxide	CO_2	0.00	0.26	2,624.39	7,281.63	72.82	7,208.82	5,046.17	2,162.65
Water	H_2O	90.08	0.01	83.81	83.81	0.84	82.97	0.00	82.97
Argon	Ar	0.00	0.85	8,510.42	9,122.42	91.22	9,031.19	0.00	9,031.19
Methane	CH_4	0.00	0.44	4,370.45	5,089.45	50.89	5,038.55	0.00	5,038.55
Total Flow (lb/hr)		90.08	6.05	60,502.33	115,305.00	1,153.05	114,152.00	5,046.17	109,106.00
Temperature (F)		90.00	91.83	91.83	48.26	48.26	48.26	48.26	48.26
Pressure (psia)		334.00	200.00	200.00	140.00	140.00	140.00	140.00	140.00
Vapor Frac		0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Enthalpy (Btu/lb)		-6,807.60	30.01	30.01	56.71	56.71	56.71	-3849.86	237.37

The table gives the component mass flow rates for the conversion of ethylene into ethylene oxide. Stream S-101 represents the starting ethylene of this process, which has a flow rate of 17,916 lb/hr. S-102 represents oxygen, which has a flow rate of 14,769.8 lb/hr. S-132, which is the recycle stream consisting of unreacted ethylene, oxygen, and side products, joins the other streams in the mixer. The mixed stream S-103 is heated by H-101 to enter the reactor at 482 F and 290.075 psia. This reactor results in a total of 141,790 lb/hr output flow rate, and contains the product ethylene oxide and a large amount of side products and unreacted ethylene and oxygen.

Then this stream enters a series of columns for purification. The stream S-108, the products from the reactor, enters D-101, and S-109, a stream of water at about 243,615. The water acts as EO absorber. A large amount of the side products escape through S-111, while most of the EO, remaining ethylene, oxygen, and side products, and water are released through S-110. D-102, the EO stripping column, removes a large amount of water at 144,211 lb/hr through S-112, while the rest of the water, EO, and other compounds are released as S-113 at a rate of 99,403.8 lb/hr. Stream S-113 enters the distillation column D-103, and through S-115 ethylene oxide and water leave as bottoms products, while the other compounds leave through as distillates through S-116. Then D-104 separates water and EO, so that EO proceeds to the carbonylation step at a rate of 24,393.1 lb/hr.

The remaining water, at 20,206.4 lb/hr, mixes with S-112. 18,206.6 lb/hr of the mix is recycled to enter D-101, 2177.61 lb/hr is purged through S-121, and the rest enters the CO_2 scrubbing process with the distillate streams from S-111 and S-116. 70% of CO_2 was scrubbed, to produce 5046.17 lb/hr of CO_2; this was an assumption from the report by Hammond et al (2009).

4.2 Section 200 - Carbonylation of Epoxide

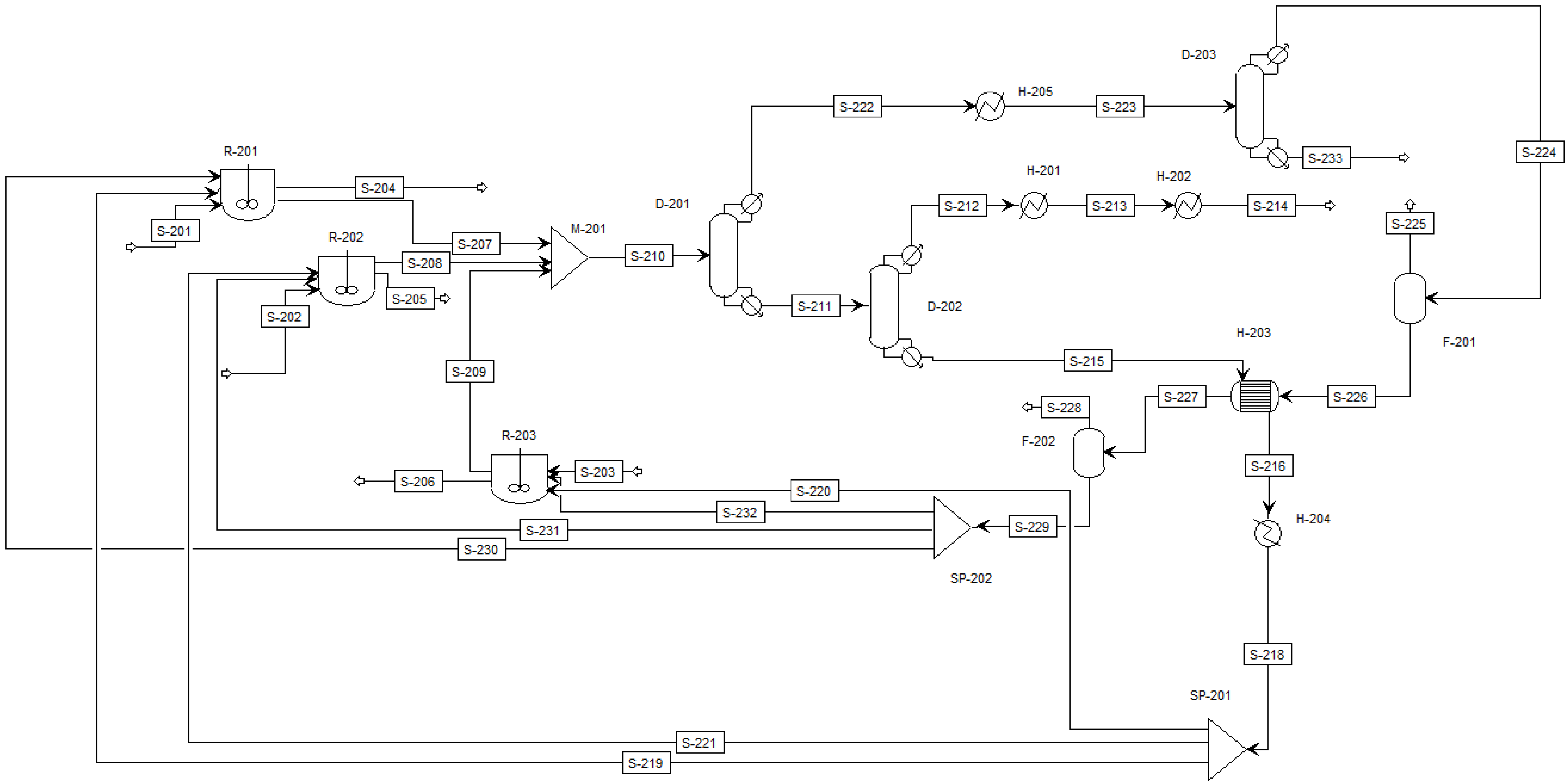


Figure 4.2

Table 4.5 Section 200 Stream Reports		**S-201**	**S-202**	**S-203**	**S-204**	**S-205**	**S-206**	**S-207**	**S-208**
		lb/hr							
Component	**Chemical Formula**								
Carbon Monoxide	CO	6,606.11	14.85	0.00	6,606.11	14.85	0.00	6,606.11	14.85
Propiolactone	C_3H_3O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene Oxide	C_4O	7,897.83	778.29	0.00	7,897.83	778.29	0.00	7,897.83	778.29
Sulfolane	$C_4H_8O_2S$	0.00	0.00	225,896.00	0.00	0.00	225,896.00	0.00	0.00
Acetaldehyde	C_2H_4O	78.98	140.97	0.00	78.98	140.97	0.00	78.98	140.97
Total Flow (lb/hr)		14,582.92	934.10	225,896.00	14,582.92	934.10	225,896.00	14,582.92	934.10
Temperature (F)		176	176	176	176	176	176	176	176
Pressure (psia)		614.70	614.70	614.70	614.70	614.70	614.70	614.70	614.70
Vapor Fraction		0.70	0.00	0.00	0.70	0.00	0.00	0.70	0.00
Enthalpy (Btu/lb)		-1,107.54	-885.50	-1,546.01	-1,107.54	-885.50	-1,546.01	-1,107.54	-885.50
Density (lb/ft^3)		4.36	46.77	76.05	4.36	46.77	76.05	4.36	46.77

Table 4.6 Section 200 Stream Reports		**S-209**	**S-210**	**S-211**	**S-212**	**S-213**	**S-214**	**S-215**	**S-216**
		lb/hr							
Component	**Chemical Formula**								
Carbon Monoxide	CO	0.00	1,770.30	1,770.30	1,770.30	5,310.91	5,310.91	0.00	0.00
Propiolactone	C_3H_3O	0.00	12,479.47	12,479.47	12,479.47	37,438.40	0.73	37,437.67	37,366.74
Ethylene Oxide	C_4O	0.00	823.86	823.86	823.86	2,471.58	2,471.58	0.00	0.00
Sulfolane	$C_4H_8O_2S$	225,896.00	225,896.00	225,896.00	225,896.00	677,689.00	0.00	677,689.00	118.88
Acetaldehyde	C_2H_4O	0.00	443.39	443.39	443.39	1330.16	1330.16	0.00	0.00
Total Flow lb/hr		225,896.00	241,413.00	241,413.00	241,413.00	724,240.00	9,113.38	715,126.00	37,485.62
Temperature (F)		176	176	176	176	176	-12.6903	449.7044	236.3227
Pressure (psia)		614.70	614.70	614.70	614.70	614.70	3.70	6.85	2.00
Vapor Fraction		0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00
Enthalpy (Btu/lb)		-1,546.01	-1,564.30	-1,564.30	-1,564.30	-1,564.30	-1,394.24	-1,444.46	-1,644.41
Density (lb/ft^3)		76.05	74.13	74.13	74.13	74.13	0.03	66.65	0.02

Table 4.7 Section 200 Stream Reports		**S-217**	**S-218**	**S-219**	**S-220**	**S-221**	**S-222**	**S-223**	**S-224**
		lb/hr							
Component	**Chemical Formula**								
Carbon Monoxide	CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propiolactone	C_3H_3O	37,366.74	37,366.74	70.93	70.93	70.93	0.07	70.86	0.00
Ethylene Oxide	C_4O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Sulfolane	$C_4H_8O_2S$	118.88	118.88	677,570.00	677,570.00	677,570.00	677.57	676,892.00	677.57
Acetaldehyde	C_2H_4O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Flow (lb/hr)		37,485.62	37,485.62	677,641.00	677,641.00	677,641.00	677.64	676,963.00	677.57
Temperature (F)		213.34	100.00	465.46	464.52	176.00	176.00	176.00	176.00
Pressure (psia)		2.00	2.00	3.50	614.70	614.70	614.70	614.70	614.70
Vapor Fraction		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Enthalpy (Btu/lb)		-1,909.34	-1,958.05	-1,418.11	-1,418.56	-1,546.05	-1,546.05	-1,546.05	-1,546.01
Density (lb/ft^3)		66.42	70.51	66.85	66.88	76.05	76.05	76.05	76.05

Table 4.8 Section 200 Stream Reports		**S-225**	**S-226**	**S-227**	**S-228**	**S-229**	**S-230**	**S-231**	**S-232**
		lb/hr							
Component	**Chemical Formula**								
Carbon Monoxide	CO	0.00	0.00	0.00	5,310.91	5,310.91	140.53	140.53	44.64
Propiolactone	C_3H_3O	23.62	23.62	23.62	0.73	0.00	0.00	0.00	0.00
Ethylene Oxide	C_4O	0.00	0.00	0.00	2,471.58	2,404.86	2,365.89	2,365.89	2,334.17
Sulfolane	$C_4H_8O_2S$	225,857.00	225,857.00	225,857.00	0.00	0.00	0.00	0.00	0.00
Acetaldehyde	C_2H_4O	0.00	0.00	0.00	1,330.16	431.94	427.96	427.96	423.84
Total Flow lb/hr		225,880.00	225,880.00	225,880.00	9,113.38	8,147.72	2,934.39	2,934.39	2,802.65
Temperature (F)		176.00	176.00	176.00	-22.76	12.76	-4.00	176.00	176.00
Pressure (psia)		614.70	614.70	614.70	17.00	14.70	614.70	614.70	614.70
Vapor Fraction		0.00	0.00	0.00	0.77	1.00	0.00	0.06	0.00
Enthalpy (Btu/lb)		-1,546.05	-1,546.05	-1,546.05	-1,482.63	-1,361.94	-1,013.12	-908.31	-885.89
Density (lb/ft^3)		76.05	76.05	76.05	0.16	0.09	55.17	27.44	46.77

Table 4.9 Section 200 Stream Reports		**S-233**	**S-234**	**S-235**	**S-236**	**S-237**	**S-238**
		lb/hr					
Component	**Chemical Formula**						
Carbon Monoxide	CO	14.88	14.88	14.88	0.00	5,170.38	95.89
Propiolactone	C_3H_3O	0.00	0.00	0.00	0.73	0.00	0.00
Ethylene Oxide	C_4O	778.06	778.06	778.06	66.72	38.97	31.72
Sulfolane	$C_4H_8O_2S$	0.00	0.00	0.00	0.00	0.00	0.00
Acetaldehyde	C_2H_4O	141.28	141.28	141.28	898.22	3.98	4.13
Total Flow (lb/hr)		934.22	934.22	934.22	965.67	5,213.33	131.74
Temperature (F)		176.00	176.00	176.00	92.89	-4.00	176.00
Pressure (psia)		614.70	614.70	614.70	16.95	614.70	614.70
Vapor Fraction		0.00	0.00	0.00	0.00	1.00	1.00
Enthalpy (Btu/lb)		-885.89	-885.89	-885.89	-1,828.07	-1,707.74	-1,385.18
Density (lb/ft^3)		46.77	46.77	46.77	47.96	3.53	2.80

The table gives the component mass flow rates for the carbonylation of ethylene oxide. Streams S-201, S-204, and S-207 represent the material that is entering this process. The total amount of input reactant mass to each CSTR is 14582.9 lb/hr. Stream S-202, S-205, and S-208 represent the recycle stream, and each of their total amounts is 934.103 lb/hr. S-203, S-206, and S-209 each contain 225,896 lb/hr sulfolane.

The total product stream, which is 724240 lb/hr, enters the distillation column D-201. The heavy components, β-propiolactone and sulfolane, leave as the bottoms product at a rate of 715126 lb/hr, while the light key, consisting of unreacted CO, ethylene oxide, and acetaldehyde, leave as distillate at a rate of 9113.38/hr.

Distillation column D-202 separates β-propiolactone from sulfolane, producing 37485.6 lb/hr of β-propiolactone that go through condensation and cooling before entering step 3. Sulfolane is heated up, split into three separate streams, and recycled back into the reactors.

D-203 removes the waste byproduct acetaldehyde and small amounts of ethylene oxide at a rate of 965.666 lb/hr. The remaining CO and EO leave as distillate at 8147.72 lb/hr. Of these, 5213.33 lb/hr of CO is evaporated by F-201 and is sent to the CO supply line. The remaining EO and small amounts of CO, at 2934.39 lb/hr, goes through one more round of heating and distillation. This leaves 2802.65 lb/hr of combined EO and small amounts of CO and acetaldehyde to return to the reactors.

Throughout the process, it is also assumed that there is 2,173 lb/hr of catalyst that circulates into the reactors and back out to be recycled with the sulfolane. Because 0.1% of sulfolane is purged to remove any side products such as succinic anhydride, replacement sulfolane and catalyst are put back into the process at a rate of 677.57 lb/hr sulfolane and 2.173 lb/hr catalyst.

4.3 Section 300 - Acid Catalyzed Rearrangement

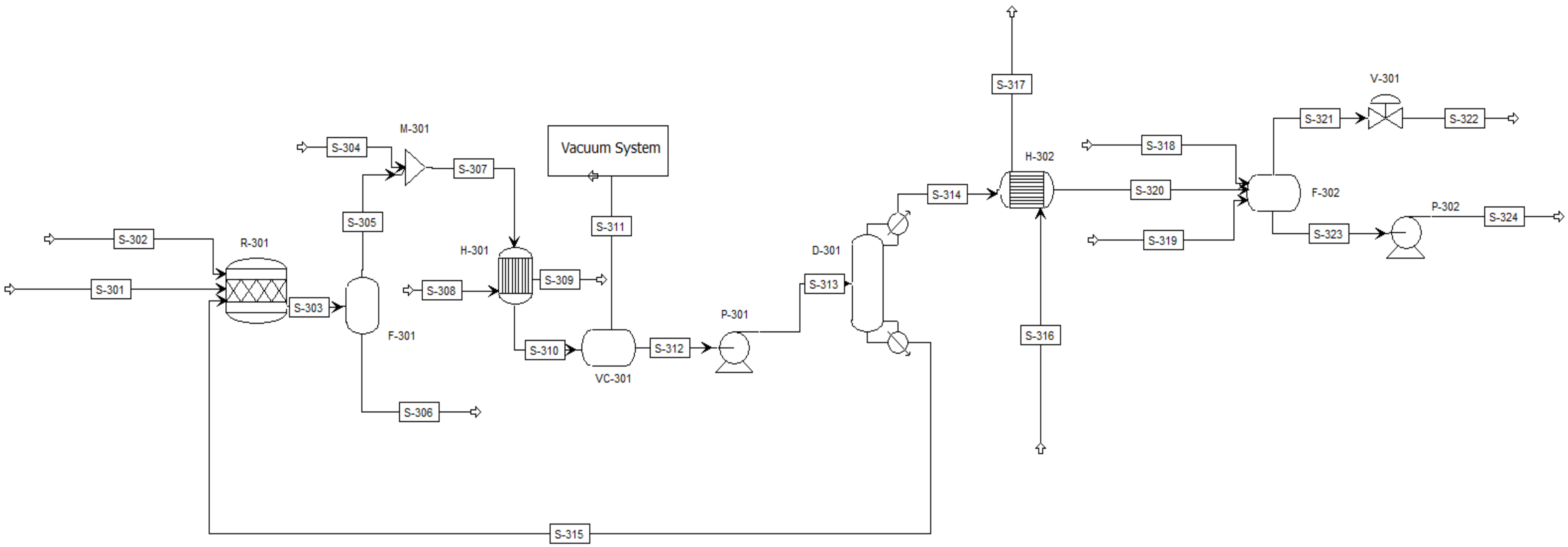


Figure 4.3

Table 4.10 Section 300 Stream Reports		**S-301**	**S-302**	**S-303**	**S-304**	**S-305**	**S-306**	**S-307**	**S-308**
		lb/hr							
Component	**Chemical Formula**								
Nitrogen	N_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
β-Propiolactone	$C_3H_4O_2$	11.40	37,313.00	1,148.74	0.00	1,137.33	11.41	1,137.33	0.00
Phosphoric Acid	H_3PO_4	4,707.21	0.00	4,707.21	0.00	0.00	4,707.21	0.00	0.00
Water	H_2O	0.00	0.00	0.00	16.21	0.00	0.00	16.21	120,000.00
Acrylic Acid	$C_3H_4O_2$	202.26	0.00	37,719.98	0.00	37,515.60	204.38	37,515.60	0.00
MEHQ	$C_7H_8O_2$	0.00	0.00	111.02	12.41	98.60	12.42	111.01	0.00
Total Flow (lb/hr)		4,920.87	37,313.00	43,686.95	28.63	38,751.52	4,935.42	38,780.15	120,000.00
Temperature (F)		338.00	100.00	338.00	194.00	338.00	338.00	336.45	90.00
Pressure (psia)		1.93	1.93	1.93	15.00	1.93	1.93	1.93	73.48
Vapor Fraction		0.00	0.00	0.91	0.00	1.00	0.00	1.00	0.00
Enthalpy (Btu/lb)		-5,306.56	-1,959.26	-2,301.33	-4,254.59	-1,920.14	-5,294.31	-1,921.86	-6,807.60
Density (lb/ft^3)		43.87	70.50	0.02	63.76	0.02	43.91	0.02	61.61

Table 4.11 Section 300 Stream Reports		**S-309**	**S-310**	**S-312**	**S-313**	**S-314**	**S-315**	**S-316**	**S-317**
		lb/hr							
Component	**Chemical Formula**								
Nitrogen	N_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
β-Propiolactone	$C_3H_4O_2$	0.00	1,137.33	1,137.33	1,137.33	170.42	966.90	0.00	0.00
Phosphoric Acid	H_3PO_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water	H_2O	120,000.00	16.21	16.21	16.21	16.21	0.00	126,107.00	126,107.00
Acrylic Acid	$C_3H_4O_2$	0.00	37,515.60	37,515.60	37,515.60	37,140.44	375.16	0.00	0.00
MEHQ	$C_7H_8O_2$	0.00	111.01	111.01	111.01	0.00	111.02	0.00	0.00
Total Flow lb/hr		120,000.00	38,780.15	38,780.15	38,780.15	37,327.08	1,453.08	126,107.00	126,107.00
Temperature (F)		160.99	175.00	175.00	175.83	346.34	386.66	90.00	161.06
Pressure (psia)		73.48	1.93	1.83	40.75	38.00	42.10	73.48	73.48
Vapor Fraction		0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
Enthalpy (Btu/lb)		-6,735.69	-2,144.38	-2,144.38	-2,144.14	-1,929.73	-1,823.29	-6,807.60	-6,735.61
Density (lb/ft^3)		59.16	61.62	61.62	61.59	0.32	57.81	61.61	59.16

Table 4.12 Section 300 Stream Reports		**S-318**	**S-319**	**S-320**	**S-323**	**S-324**
		lb/hr				
Component	**Chemical Formula**					
Nitrogen	N_2	5.00	0.00	0.00	5.00	5.00
β-Propiolactone	$C_3H_4O_2$	0.00	0.00	170.42	170.42	170.42
Phosphoric Acid	H_3PO_4	0.00	0.00	0.00	0.00	0.00
Water	H_2O	0.00	16.21	16.21	32.43	32.43
Acrylic Acid	$C_3H_4O_2$	0.00	0.00	37,140.44	37,140.44	37,140.44
MEHQ	$C_7H_8O_2$	0.00	12.41	0.00	12.41	12.41
Total Flow (lb/hr)		5.00	28.63	37,327.08	37,360.70	37,360.70
Temperature (F)		90.00	80.00	100.00	100.04	100.60
Pressure (psia)		17.00	20.00	17.00	15.00	50.00
Vapor Fraction		1.00	0.00	0.00	0.00	0.00
Enthalpy (Btu/lb)		3.23	-4,342.40	-2,172.92	-2,174.29	-2,174.15
Density (lb/ft^3)		0.08	68.06	64.42	64.41	64.39

Table gives the component mass flow rates for the acid catalyzed rearrangement to acrylic acid. Stream S-301 represents the starting material of what is charged to the reactor during the start-up of the process. The stream is not fed continuously, and was only used to satisfy the mass balance requirement in Aspen plus. Stream S-302 has a mass flow rate of 37,300 lb/hr of propiolactone, and is the total propiolactone produced in the second stage of the process. Stream S-315 is the bottoms product of column D-301. The stream is pure liquid with a temperature of 386 ^{o}F and a total mass flow rate of 1,453 lb/hr. S-315 feeds back into the reactor R-301, replacing 970 lb/hr of unreacted propiolactone.

The reactor operates at a pressure of 1.93 psia with a temperature of 338 ^{o}F. The streams fed to the reactor are in the liquid phase, while the reactor products are entirely vapor. Flash Vessel F-301 allows for the separation of vapor and liquid product from the RSTOIC unit, and does not exist in the real process. Stream S-306 was added to satisfy the mass balance in Aspen plus and it contains all of the phosphoric acid added to the process, as well as trace amounts of MEHQ inhibitor. In reality, the phosphoric acid catalyst is not to cross the reactor boundaries, so S-306 will function as a small purge stream, consisting mainly of MEHQ. Stream S-305 is the vapor product stream from reactor R-301, consisting of un-reacted β-propiolactone. This stream is then mixed with a feed of MEHQ inhibitor, S-304. Following the reaction zone, S-307 is cooled from 336 to 175 ^{o}F prior to applying a vacuum of 1.93 psia. Condensing the vapors minimizes the amount of product loss.

Acrylic acid enters the distillation column D-301 on tray 7 at a pressure of 40.75 psia. This pressure increase allows for a lower operating temperature of the condenser of the column. Stream S-314 is the vapor product from the column and contains acrylic acid with a mass purity of 99.4%. The flow rate is 37,327 lb/hr with a temperature of 346.34 ^{o}F. The main impurity of this stream is 170 lb/hr of β-propiolactone. Streams S-319 and S-318 are combined with the overhead product. S-319 contains 10% MEHQ on a molar basis with the balance of water. S-318 supplies nitrogen to flash vessel F-302 in order to maintain operation at atmospheric pressure. The final acrylic acid product is pumped to a pressure of 50 psia for storage with an MEHQ concentration of 300 ppm.

Section 5 – Energy Balance and Utilities

Table 5.1	**Inlet Streams**			**Outlet Streams**				
lbmol/hr	**S-101**	**S-102**	**S-125**	**S-118**	**S-121**	**S-126**	**S-129**	**S-131**
Ethylene	636.80	0.00	0.00	0.00	0.01	0.09	24.49	0.00
Oxygen	0.00	458.70	0.00	0.00	0.00	0.06	6.36	0.00
Ethylene Oxide	0.00	0.00	0.00	550.94	0.03	0.00	0.03	0.00
Formaldehyde	0.00	0.00	0.00	1.50	0.06	0.00	1.51	0.00
Acetaldehyde	0.00	0.00	0.00	1.53	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.01	1.65	114.66
Water	0.00	0.00	10.00	0.56	125.71	0.00	0.05	0.00
Argon	0.00	2.31	0.00	0.00	0.00	0.02	2.28	0.00
Methane	3.20	0.00	0.00	0.00	0.00	0.03	3.17	0.00
Total Flow lb/hr	17,915.97	14,769.77	180.15	24,393.06	2,267.74	6.05	1,153.00	5,046.17
Enthalpy Btu/hr	14,793,400.00	244,876.00	-1,226,400.00	-12,801,000.00	-14,784,000.00	180.60	65,361.35	-19,000,000.00
Differences								
Total Flow lb/hr		0.13						
Enthalpy Btu/hr		-60,758,334.00						

Table 5.2	**Inlet Streams**					**Outlet Streams**			
lbmol/hr	**S-201**	**S-204**	**S-207**	**S-224**	**S-218**	**S-222**	**S-236**	**S-237**	**S-238**
Carbon monoxide	235.84	235.84	235.84	0.00	0.00	0.00	0.00	184.59	3.42
β-propiolactone	0.00	0.00	0.00	0.00	518.52	0.00	0.01	0.00	0.00
Ethylene oxide	179.28	179.28	179.28	0.00	0.00	0.00	1.52	0.88	0.72
Sulfolane	0.00	0.00	0.00	5.64	0.99	5.64	0.00	0.00	0.00
Acetaldehyde	1.79	1.79	1.79	0.00	0.00	0.00	20.39	0.09	0.09
Total Flow lb/hr	14,582.92	14,582.92	14,582.92	677.57	37,485.61	677.64	965.67	5,213.33	131.74
Enthalpy Btu/hr	-16,200,000.00	-16,200,000.00	-16,200,000.00	-1,050,000.00	-71,600,000.00	-1,050,000.00	-1,770,000.00	-8,900,000.00	-182,490.00
Difference									
Total Flow lb/hr	47.66								
Enthalpy Btu/hr	-33,970,990.00								

Table 5.3	**Inlet Streams**					**Outlet Streams**		
lbmol/hr	**S-301**	**S-302**	**S-304**	**S-318**	**S-319**	**S-306**	**S-322**	**S-324**
Nitrogen	0.00	0.00	0.00	0.18	0.00	0.09	0.00	0.18
β-propiolactone	0.16	517.78	0.00	0.00	0.00	0.06	0.00	2.36
Phosphoric Acid	48.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water	0.00	0.00	0.90	0.00	0.90	0.00	0.00	1.80
Acrylic Acid	2.81	0.00	0.00	0.00	0.00	0.00	0.00	515.38
MEHQ	0.00	0.00	0.10	0.00	0.10	0.01	0.00	0.10
Total Flow lb/hr	4,920.87	37,313.00	28.63	5.00	28.63	4,935.43	0.00	37,360.70
Enthalpy Btu/hr	-26,112,912.00	-73,105,906.00	-121,799.10	16.14	-124,312.80	-26,129,671.00	0.00	-81,000,000.00
Difference								
Total Flow lb/hr	0.00							
Enthalpy Btu/hr	-7,892,487.00							

Table 5.4. Utility Requirements

	Name	**Fluid**	**Rate**	**Rate Units**
STEP 1	Electricity		162.355	KW
	Cooling Water	Water	507175	GAL/H
	Process Water Start Up	Water	22525	GAL
	Process Water	Water	22.525	GAL/H
	Refrigerant - Propane	Refrigerant	261.3359	KLB/H
	Refrigerant - Freon 12	Refrigerant	1064.454	KLB/H
	Steam @100PSI	Steam	108.3391	KLB/H
	Steam @165PSI	Steam	86.3409	KLB/H
STEP 2	Electricity		898.235	KW
	Cooling Water	Water	712617	GAL/H
	Refrigerant - Propane	Refrigerant	4.74008	KLB/H
	Refrigerant - Freon 12	Refrigerant	48.5794	KLB/H
	Steam @100PSI	Steam	4.60524	KLB/H
STEP 3	Electricity		80.668	KW
	Cooling Water	Water	46170	GAL/H
	Steam @400PSI	Steam	20.71821	KLB/H

The large enthalpy difference between input and output reflect the need for heat input or output. Step 1 is endothermic, while step 2 and 3 are exothermic. Heat exchangers have been installed throughout the process to meet these energy requirements.

The entire process requires a large amount of water, in total 1,265,962 gallons per hour. The main consumers of cooling water are the heat distillation towers' condensers and other heat exchangers that are in steps 1 and 2. Step 3 only has one distillation tower and it does not need to produce a large amount of condensation due to its comparatively smaller size.

Electricity total is 1,141.258 kW. Steps 1 and 3 only have pumps, which require less electricity to operate, but step 2 contains a compressor, which requires a larger amount of electricity.

Although the need to cool to very low temperatures is present both steps 1 and 2, the refrigerant costs are much higher in step 1. This is due to the fact that streams that must be cooled with refrigerants are much larger in step 1 than in step 2. For example, in heat exchanger H-105, the total flow rate of water is 18,026.6 lb/hr at 1 degree Fahrenheit, and H-104 produces a stream that is 99,403.8 lb/hr at -28.64 degrees Fahrenheit. In contrast, the refrigerant-cooled stream S-214 is has only 9113.38 lb/hr flow rate, and S-229 at 8147.72 lb/hr. The lack of refrigerants in step 3 is expected, as none of the condensers or coolers reach very low temperatures.

The process water in step 1 accounts for the water needed in the scrubbing of ethylene oxide. Although a larger amount of it is required to start up the process, only a small amount is needed after the process has been started.

Section 6 – Economic Analysis

6.1 Overview

The economics of this project are heavily dependent on the cost of ethylene oxide. A microchannel reactor was used in an effort to save on capital and utility costs. However, the ethylene oxide process may not accurately represent the process that is seen in industry. For this reason, three separate economic analyses were conducted. The first section contains economics based on the entire process. The second contains economics regarding each independent process, calculated as if each plant were to be built separately. The third contains economics using a cost-plus analysis of ethylene oxide along with a sensitivity analysis on the market price for ethylene oxide; this is referred to as the two-step process with EO as the raw material. The excel spreadsheets used for these calculations can be found in the appendix. The life of the plant was assumed to be 35 years. Calculation assumptions are listed at the end of this section.

6.2 Total Project

The total capital investment (C_{TCI}) for the entire project is $559,236,766.35. This capital investment is quite large are variable due to the Ethylene oxidation part of the project. Capital costs for the microchannel reactor and the CO_2 scrubbing unit were based off of the costs calculated from *Alaskan Natural Gas to Liquids* and could play a huge role in the profitability of the plant. The total utility costs were calculated to be $12,435,933.93 per year, while the total fixed costs and variable costs per year were $78,297,468.99 and $124,792,455.72, respectively. An after tax cash flow analysis was conducted, and at an assumed ethylene price of $.46/lb, acrylic acid selling price at $1.00/lb, and an after tax discount rate of 15%, the NPV was calculated to be a loss of $48,174,085.70 with an IRR of 13.84%, below the threshold of 15%. For the purposes of this economic analysis, costs were assumed as follows: Ethylene $0.46/lb, Oxygen $0.05/lb, CO2 Removal solvents and MEA $0.31/barrel EO, Carbon Monoxide $0.10/lb, and MEHQ $5.00/lb. The cash flow analysis and calculations can be found in the appendix.

6.2.1 Sensitivity Analysis: Market Price of Ethylene

The biggest single contributor to the cost of the Acrylic Acid plant is the cost of ethylene, accounting for 70M of the 190M total yearly costs. Currently, the price of ethylene is assumed to be the price listed by ICIS. The price for pipeline ethylene ranges from $.46 to $.70. However, with the huge recent boom in natural gas drilling due to hydrofracturing and the announcement of the construction of major ethane crackers, the price is expected to fall. A sensitivity analysis has been constructed to grasp the effect of cheap natural gas on acrylic acid production and its potential to knock off propylene-based producers. As seen in table, the minimum ethylene price would have to be $.41 to break even. Also, a decrease in ethylene price by $.15 or almost 35% could increase the IRR by merely 3.5%. This is a feasible decrease in ethylene costs which could be realized when the operation of newly announced ethane crackers start producing by 2018. However, it is evident that the initial capital investment is so large that the plant does not accumulate a reasonable profitability over the course of 35 years.

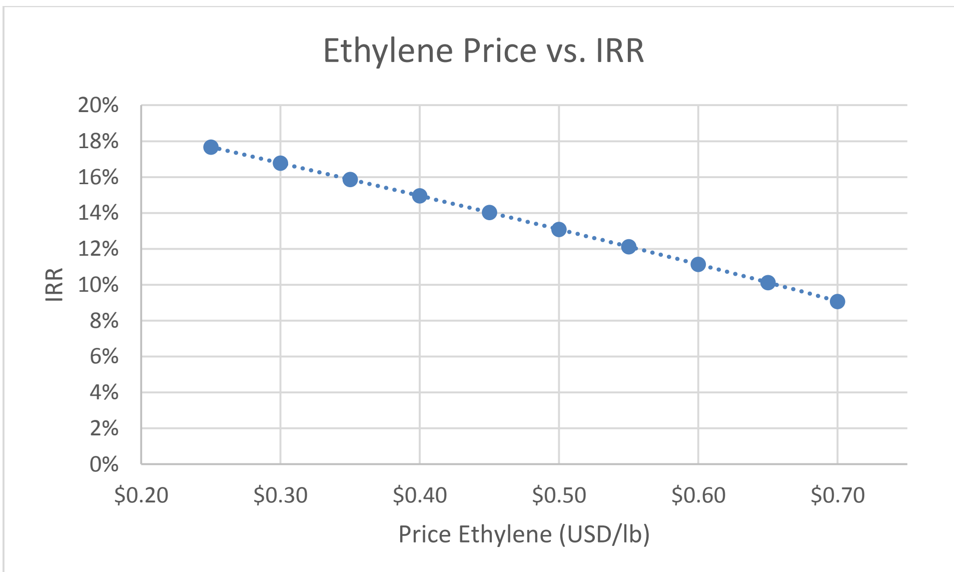


Figure 6.1

6.2.2 Sensitivity Analysis: Total Capital Investment

As seen in the analysis above, the plant is barely profitable even with a 35% decrease in ethylene price due in large part to the capital investment of the plant. Below is a sensitivity analysis on the change in TCI vs. IRR which is conducted due to the high level of assumptions and variability in design and costing. Decreasing capital costs can increase the IRR significantly, while increasing capital costs do not decrease the IRR as rapidly. A mere decrease in TCI by 10% to $510M causes an increase in the IRR to the 15% threshold. This shows that the profitability is extremely dependent on the capital costs of the EO portion of the plant, considering that the EO equipment alone account for 50% of total capital investment costs and 90% of all plant equipment costs. This promotes the idea that the microchannels are not cost beneficial. Despite the amount they save in yearly utilities, the initial investment is too great. A further analysis is conducted for the 2-step process to determine the savings on scrapping the EO portion of the plant.

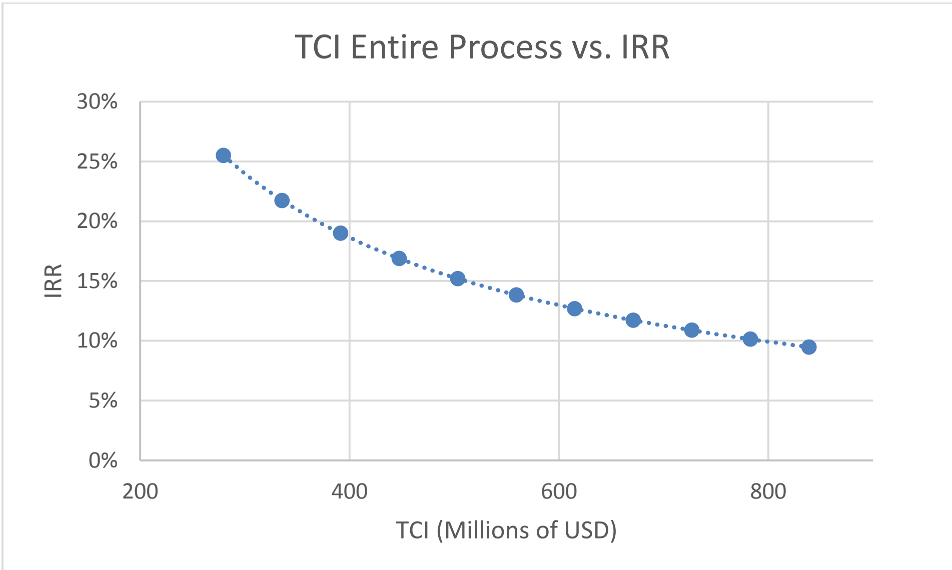


Figure 4

6.2.3 Sensitivity Analysis: Acrylic Acid Sale Price

Currently, acrylic acid sells at \$.84 to \$.90 per pound via pipeline and \$1.09 to \$1.12 per pound packaged. If the market continues to grow, prices could drop as large chemical producers join in the production in the US due to low potential raw material costs by increasing the supply. Alternatively, as the world continues to increase their use of plastics and polymers, the demand for acrylic acid could increase significantly and push up prices. A sensitivity analysis is done on the sale price of acrylic acid to account for these possibilities. It was determined that the breakeven market price of acrylic acid would have to be \$1.04. A 30% increase in price can increase the IRR by 12%. However, even a drop of 25% on costs could put the project at a negative IRR. As demand for acrylic acid continues to rise, fluctuating prices are expected to play a huge role in the profitability of the plant. Thus, this analysis does not justify the building of the entire plant.

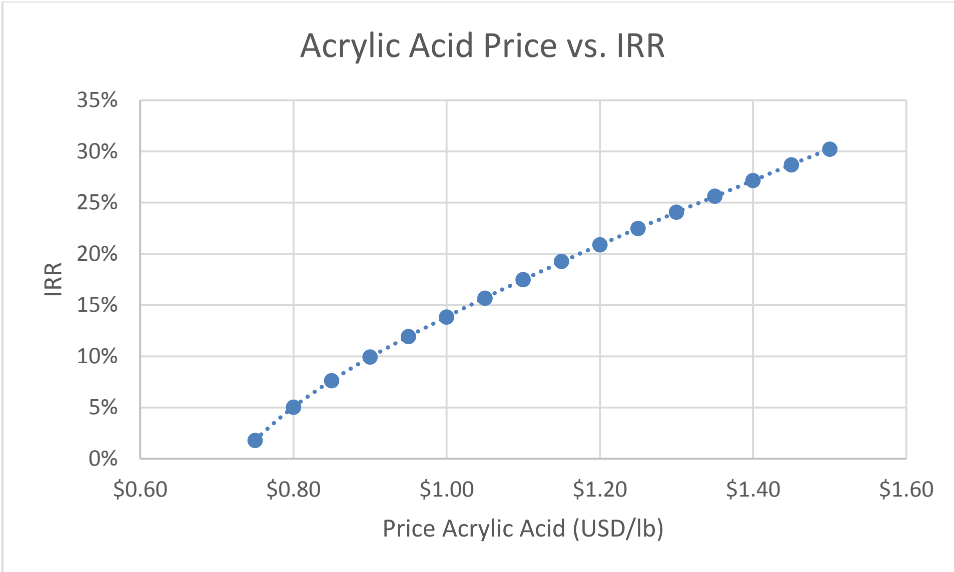


Figure 6.3

6.3 Individual Processes

Below, economic analyses are offered for each individual plant. This was conducted to get a better idea on which processes are feasible, especially whether or not ethylene oxide should be purchased from the market or produced.

6.3.1 Ethylene Oxide Process

The total capital investment for block 100 is $487,300,037.08, an enormous amount for an ethylene oxide plant and clearly the largest investment of all three processes. Total utilities for this section are $9,890,768.60. The total fixed costs and variable costs were calculated to be $67,475,247.22 and $93,949,931.06, respectively. The total variable revenue is merely $152,633,250.00, resulting in an NPV and total loss of $585,350,578.54 after 35 years of operation. This data alone proves that the EO process is not profitable nor viable. With the microchannel reactors costing $135M, it is clear that the price of the reactor overshadows and potential advantages that could be offered.

6.3.2 Carbonylation Process

The total capital investment for block 200 is $107,005,039.00, a much smaller investment compared to the EO plant. Total utilities for this section are $1,137,805.72, much less than the

EO plant and less than 10% of the entire process utilities. The total fixed costs and variable costs were calculated to be $10,430,577.23 and $197,300,477.30, respectively. The high variable cost is due to the necessity to purchase ethylene oxide and market prices. The total variable revenue is $266,772,605.40, resulting in an NPV of $179,582,851.13 after 35 years of operation with an IRR of 34.72%.

6.3.3 Rearrangement Process

The total capital investment for block 300 is $81,000,956.30. Total utilities are $1,407,359.61, total fixed costs are $6,089,833.62, and total variable costs are $303,276,605.40. It is important to note that the total variable costs are high because this process assumes that β-propiolactone is purchased on the market at a price that is between the price of EO and acrylic acid. This is not accurate, however, because β-propiolactone is not a produced in bulk like most market commodity chemicals. The total variable revenue is $300,000,000.00, resulting in an NPV of -$155,980,809.87 after 35 years of operation.

6.3.4 Individual Process Conclusion

It is extremely important to note that a price of $.85/lb was used for β-propiolactone, which is between the market prices of EO and acrylic acid. The costing for the last two steps individually is difficult to confirm since there does not exist a large market for β-propiolactone. However, the economic analysis on the first process, the EO plant, clearly shows that the microchannel reactors are too costly to build and maintain to overcome the advantages offered such as the reduced amount of inerts and diluents present.

Based on total yearly operating costs, including total yearly utilities, operating costs, oxygen costs, and fixed costs, the cost of production of ethylene oxide is $77M. This results in a markup of $.45 per pound of ethylene. This was calculated by doing an economic analysis on the individual EO plant. When added to the ethane market price of $.46, it was determined that the cost-plus price of EO was $.91, significantly above the current EO prices. This led to the realization that the EO plant built is not profitable, too expensive, and simply not profitable. The spreadsheets can be found in the appendix.

It is clear that EO should be purchased from the market, and that the 2-step process should be further analyzed for profitability.

6.4 Two-Step Process

The total capital investment (C_{TCI}) for blocks 200 and 300 is $120,274,816.16, a significantly smaller sum than with the EO plant. The total utility costs were calculated to be $2,545,165.33 per year, around 80% less than with the EO plant while the total fixed costs decreased by almost 82% to $13,357,182.62 per year. The variable costs increased by 60% to $201,791,764.66 because of the ethylene oxide prices that were assumed. Ethylene oxide sells for $.74 to $.79 per pound, so a median of $.75 was assumed for these calculations.

An after tax cash flow analysis was conducted with the assumed ethylene oxide price of $.76 and the assumed ethylene price of $.46/lb. With an after tax discount rate of 15%, the NPV was calculated to be $287,456,509.12 with an IRR of 42.17% The cash flow analysis and calculations can be found in the appendix.

It is difficult to determine the mark-up which suppliers tack on to their ethylene oxide price, and it is evident that the oxidation step accounts for the greatest cost of production out of the three. However, at the production rate of 300M pound per year which only accounts for 3% of the current world production of acrylic acid and 2.15% by 2018, it may not be worth building a separate epoxidation section to the acrylic acid plant. The purpose of this analysis is to get an idea of how sensitive profits are to the markup of ethylene oxide.

6.4.1 Sensitivity Analysis: Market Price of Ethylene Oxide

The biggest single contributor to the cost of the 2-step process is ethylene oxide. Currently, the price of ethylene is assumed to be the price listed by ICIS. A sensitivity analysis has been constructed to grasp the effect of ethylene oxide price. The minimum breakeven price of ethylene oxide would have to be $1.05/lb, well above the ICIS market price of $.75/lb. A decrease in ethylene oxide price by 20% leads to an increase in IRR by 12% while a 20% price increase leads to a decrease in IRR by 12%, demonstrating the huge dependence EO price plays in the profitability of this plant. This motivates the idea that pricing stability and long-term contracts would be necessary to take advantage of the potential profitability of the 2-step process.

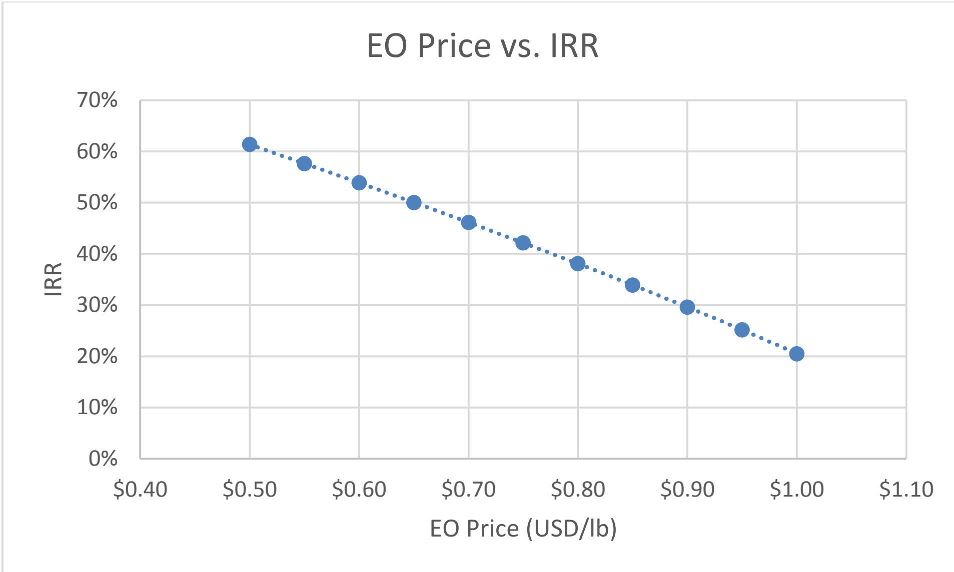


Figure 6.4

6.4.2 Sensitivity Analysis: Total Capital Investment

Below is a sensitivity analysis on the change in total capital investment cost vs. IRR. The curved nature of this analysis shows that a decrease in TCI will have a greater impact than an Increase in TCI. The 2-step process is inherently cheaper than the entire process by 80%. This leads to large prospects of profitability; when the TCI is increased by 30%, the IRR drops by 10%, but increases by 15% when TCI is decreased by 30%. The breakeven TCI cutoff would have to be an incredible $408M, more than triple the projected TCI. If the project is constructed, TCI is sure to increase, however, this sensitivity analysis shows that a major increase in TCI can still be offset due to the profitability of this plant. If coupled with increasing demand and market prices of acrylic acid, the previous statement could indeed hold.

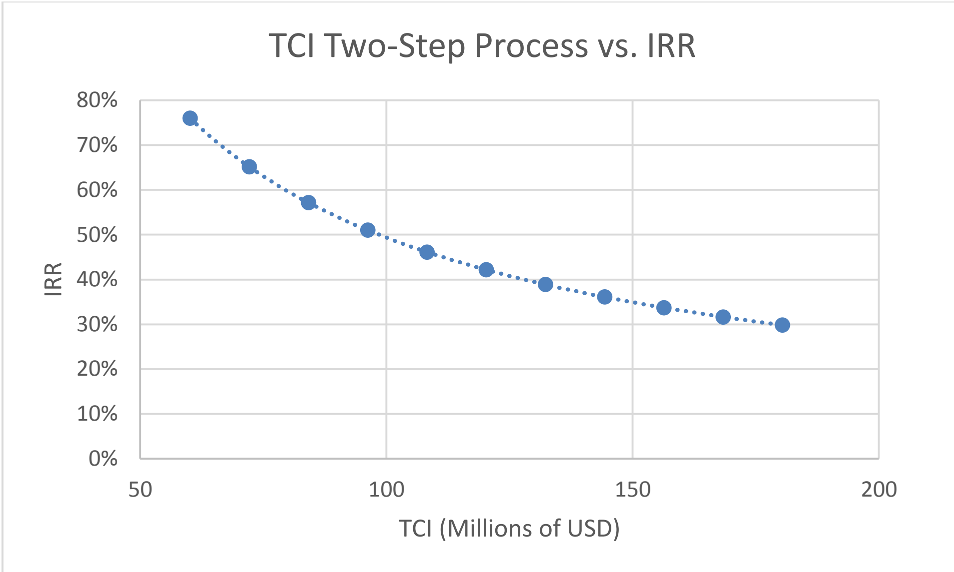


Figure 6.5

6.4.3 Sensitivity Analysis: Acrylic Acid Sale Price

A sensitivity analysis was conducted on the sale price of acrylic acid on the 2-step process. It was determined that the breakeven market price of acrylic acid would have to be \$.76, significantly lower than current prices and 2006 ICIS prices. A 10% increase in price can increase the IRR by 10%. However, a drop of 10% on acrylic acid price could decrease the IRR by 12%. As demand for acrylic acid continues to rise, fluctuating prices are expected to play a huge role in the profitability of the plant. Thus, this analysis does not justify the building of the entire plant.

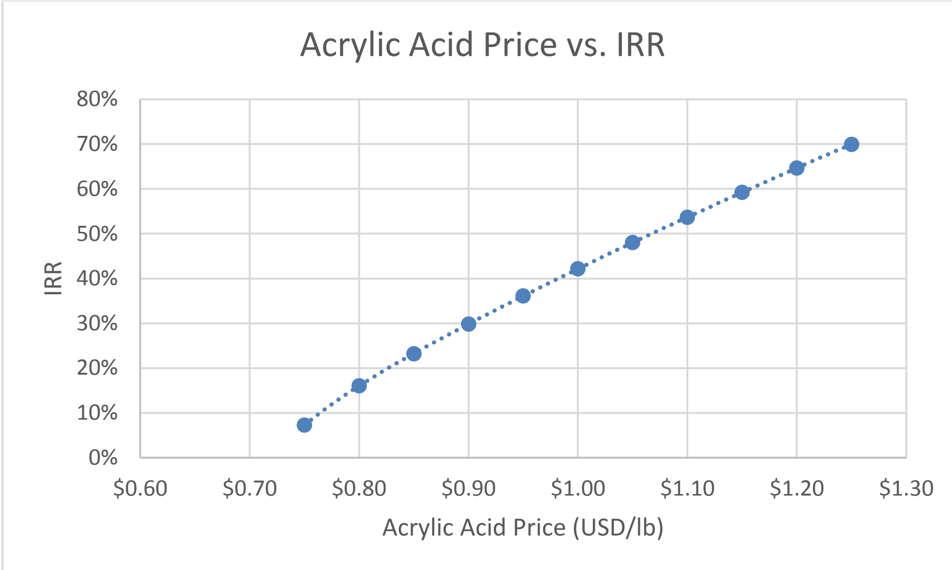


Figure 6.6

6.4.4 Sensitivity Analysis: Acrylic Acid Market Price vs. Ethylene Oxide Market Price

Below is a chart relating the change in ethylene oxide price and acrylic acid price to understand how the highly market dependent, 2-step process would fare. The IRRs in green indicate profitability with a ladder separating profitable market price combinations vs. non-profitable market price combinations.

Table 6.1 *IRR vs. Ethylene Market Price vs. Ethylene Oxide markup*

	$0.75	**$0.80**	**$0.85**	**$0.90**	**$0.95**	**$1.00**	**$1.05**	**$1.10**	**$1.15**	**$1.20**	**$1.25**
$0.50	32.34%	38.52%	44.48%	50.25%	55.87%	61.36%	66.75%	72.03%	77.23%	82.35%	87.41%
$0.55	27.99%	34.36%	40.46%	46.35%	52.07%	57.65%	63.11%	68.46%	73.71%	78.89%	83.99%
$0.60	23.47%	30.07%	36.35%	42.37%	48.21%	53.88%	59.42%	64.84%	70.16%	75.39%	80.53%
$0.65	18.70%	25.64%	32.12%	38.31%	44.27%	50.05%	55.68%	61.17%	66.56%	71.85%	77.05%
$0.70	13.52%	21.00%	27.76%	34.14%	40.25%	46.15%	51.87%	57.46%	62.92%	68.27%	73.53%
$0.75	7.26%	16.05%	23.23%	29.85%	36.13%	42.17%	48.01%	53.68%	59.23%	64.65%	69.97%
$0.80	NEG IRR	10.46%	18.45%	25.40%	31.90%	38.09%	44.06%	49.85%	55.48%	60.98%	66.37%
$0.85	NEG IRR	2.46%	13.23%	20.75%	27.53%	33.92%	40.04%	45.94%	51.68%	57.26%	62.73%
$0.90	NEG IRR	NEG IRR	6.87%	15.78%	22.99%	29.62%	35.91%	41.96%	47.80%	53.49%	59.03%
$0.95	NEG IRR	NEG IRR	NEG IRR	10.13%	18.19%	25.17%	31.68%	37.88%	43.86%	49.65%	55.29%
$1.00	NEG IRR	NEG IRR	NEG IRR	1.81%	12.94%	20.50%	27.30%	33.70%	39.83%	45.74%	51.48%

6.5 Calculation Assumptions

Listed below are the assumptions made during the economic analysis. The economic analysis and costing for this section was calculated using Chapter 22, *Cost Accounting and Capital Cost Estimation* and Chapter 23, *Annual Costs, Earnings, and Profitability Analysis* from *Seider et al*.

6.5.1 Total Capital Investment

A breakdown of the components included in C_{TCI} is shown in Table 22.9 of *Seider et al*. Important assumptions were made to better represent the difficulties of this process or to increase the potential profitability of this project.

First, equipment costs were calculated for plant fabricated equipment, process machinery, and storage tanks using the methods provided in Chapter 22 and by accounting for field materials, labor, and indirect module expenses related to installation with the Guthrie bare-module factors as listed in Table 22.11 in *Seider et at*. These costs were then escalated by a CE factor of 525 for 2013 to account for the inflation that occurred in the years after the 2008 recession. Spare parts were assumed to cost 20% of the total equipment costs. Computer and software costs were assumed to hover around 10% of total equipment costs. These sum to produce the Total bare-module costs (C_{TBM}).

Following this, the costs for site and services and allocated costs for utilities were calculates. It was assumed that site preparation would cost 6% of C_{TBM} since land in Texas is flat and consistent and because the plant would not be grass-root. Service facilities would be relatively cheap and were assumed to cost 5% of C_{TBM} since it is assumed that this is not a grass-root plant and that facilities would be relatively well established. Allocated cost for utility plants was calculated using Table 22.12 in *Seider, et al*. All costs were summed to calculate the direct permanent investment costs, C_{DPI}. Contingencies and contractor fees were assumed to cost 35% of C_{DPI} because this is a preliminary design report. This was then summed with C_{DPI} to get total depreciable capital, C_{TDC}. Land in Texas is relatively cheap and was assumed to cost 2% of C_{TDC}, and startup was assumed to cost a minimal 10% of C_{TDC} due to the ease of chemical work in Texas. These were summed to calculate the total permanent investment, C_{TPI}. Working capital was calculated by determining the necessary cash reserves for 30 days of raw materials, 7 days of product inventories, 30 days of accounts receivable, and 30 days of accounts payable.

It was assumed that it would take 1 year for construction and 1 year for plant startup due to the location of the project in the Texas Gulf which leads to easier access to material for construction and production away from a large population center.

6.5.2 Total Fixed Costs

Depreciation was not included in these calculations since MACRS was chosen over a straight-line method. The calculated COM is based on total utilities, labor-related operations, maintenance, operating overhead, and property taxes and insurance.

Utilities were calculated using heat transfer equations and by following the examples in *Seider et al*. This includes determining the amount of steam at 100PSI, 165PSI, and 400PSI, propane and Freon coolant, and cooling water needed. Costs for each utility are taken from *Seider et al*. and adjusted to match the assumed CE index of 2014. Utility costs for MEA are adapted from *Alaskan Natural Gas to Liquids*.

Operation wages were calculated based on operation 24 hours a day, 7 days a week. At 168 hours per week divided by an operator's 40 hours work week, 4.2 shifts are required per week. To account of sick days and vacation days, 5 shifts were chosen. Since the plant is a smaller scale acrylic acid plant, it was assumed that only 4 operators per section would be required. The method to calculating total operations annual cost follows that in Seider et al.

Total annual maintenance costs were calculated as outlined in Seider et al. However, all factors were increased by 20% of the recommended scaling to account for the fact that all the intermediate ethylene oxide is corrosive, the intermediate β-propiolactone can produce a solid that needs to be purged out of the system, and the product acrylic acid could potentially polymerize, with the byproduct needing to be removed from the system.

Operating overhead was calculated as outline in Seider et al. Property taxes and insurance was assumed to cost 2% of C_{TDC} since the process will be low risk located away from a large population in Texas where property is relatively cheap.

Depreciation is included in the cash flow analysis separate of COM. A 5-year MACRS recovery period was chosen as indicated by the IRS asset class 28.0 for the manufacture of chemicals and allied products.

6.5.3 Total Variable Costs

Total variable costs account for all marginal costs in this process and include the cost of raw materials including ethylene, oxygen, carbon monoxide, MEA reagents, MEHQ inhibitor, catalysts, and product sale general expenses. In the first year of operation, the plant will run at 50% capacity. These costs are scaled to match inflation. Utilities are not included as a variable cost because even if the plant production decreases, the cost of running utilities plants and operating utilities plants stays the same; for example, it is assumed that the boiler will constantly produce 400PSI steam.

6.5.4 Cash Flow Analysis

An after tax cash flow analysis was conducted to determine the net present value of the project. Total capital investment was treated as a cost in the 1st year of plant life. The 2nd year of plan life exhibited 50% capacity, so while fixed costs remained constant, variable costs and revenue were 50% of what their normal value was. In the 3rd year and on, the fixed and variable costs and revenue were included at their full value and inflated per year by 3%. Depreciation was treated as 5-year MACRS under the IRS asset class 28.0. Taxable income was calculated and taxed at a total rate of 40% which is estimated to account for a Federal Tax rate of 35%-37% and the state tax. An after tax cash flow was calculated per year and an NPV was calculated using an after tax discount rate of 15%.

Section 7 – Safety and Environmental Factors

7.1 Section 100

Many hazardous chemicals are used in the oxidation of ethylene stage, including formaldehyde, acetaldehyde, and methane. Formaldehyde and acetaldehyde are known carcinogens and skin irritants, and both are flammable in small amounts.

Ethylene Oxide

Ethylene oxide is a highly reactive compound due to its high ring strain. Most reactions in which it participates are highly exothermic, and involve a ring opening reaction in which ethylene oxide (EO) participates as an electrophile. As it is a known environmental pollutant, steps must be taken to contain any unreacted EO that can potentially appear in the atmosphere. This processes converts EO to lactone by an oxygen based process, leading to the possibility of EO entering the flammable region. As a result, parameters such as temperature, pressure, residence time, and composition of the EO must be carefully monitored throughout the reaction.

The primary environmental concerns in the oxidation process, with regards to side products, include the formation of ethylene, ethylene oxide, carbon dioxide and ethane. These are typically seen in the process purge following the EO scrubber. It should be further noted that the EO vapors are liable to explosive decomposition if they reach pressure greater than 300 mm Hg. Other concerns include the effect of mixing EO with air. In this case, flames can occur at much lower pressures, such as 10 to 20 mm Hg.

Ethylene oxide is toxic in both its liquid and gaseous forms. Short term exposure to moderate concentrations is linked to irritation of the respiratory system, and may cause lung injury. Due to its very low boiling temperature, EO is able to evaporate rapidly from the skin, causing burns similar to frostbite.

Methane

While methane has little toxicity, it is extremely combustible and is a known asphyxiate. Methane forms explosive mixtures in the air at atmospheric pressure. Care should be taken to monitor oxygen levels and see that they are maintained at normal levels for worker safety.

7.2 Section 200

β-Propiolactone

β-Propiolactone is a suspected human carcinogen. To improve acrylic acid yields and limit work place exposure, care will be taken to avoid its isolation.

Sulfolane

Sulfolane acts as a solvent in the second step, therefore large quantities are used throughout the process. While sulfolane has low skin penetration, it is still toxic, and care must be taken while handling it. Efforts will be made to reuse whenever possible. Special care must be taken when considering disposal.

7.3 Section 300

Phosphoric Acid

Concentrated (greater than 85 mass percent) phosphoric acid is used throughout the process. A strong mineral acid, phosphoric acid is extremely corrosive towards most types of steel and must be safely stored in glass lined containers or certain plastics. The chemical has negligible vapor pressure, so very little if any will pass the reactor boundaries except during start-up and shut down. In these situations, proper handling must be observed.

Acrylic Acid

This process produces acrylic acid at a mass flow rate of 37,000 lb/hr. The product is stored with MEHQ inhibitor at a concentration of 300 ppm in a stainless steel container with 10% air by volume. The air is necessary for the MEHQ inhibition mechanism. Acrylic acid is corrosive towards the skin and respiratory tract.

Section 8 – Equipment

8.1 Equipment List

8.1.1 Block 100

Equipment Number	Name	Type
C-101	Purification Tower 1 Reflux Drum	Fabricated Equipment
C-102	Purification Tower 2 Reflux Drum	Fabricated Equipment
D-101	EO Absorber	Fabricated Equipment
D-102	EO Stripper	Fabricated Equipment
D-103	Purification Tower 1	Fabricated Equipment
D-104	Purification Tower 2	Fabricated Equipment
H-101	Inlet Gas Heater	Fabricated Equipment
H-102	Outlet Gas Cooler	Fabricated Equipment
H-103	Purification Tower 1 Feed Stream Cooler	Fabricated Equipment
H-104	Recycle Water Cooler	Fabricated Equipment
H-105	Steam Quench Heater	Fabricated Equipment
H-106	EO Stripper Reboiler	Fabricated Equipment
H-107	Purification Tower 1 Reboiler	Fabricated Equipment
H-108	Purification Tower 2 Reboiler	Fabricated Equipment
H-109	Purification Tower 1 Condenser	Fabricated Equipment
H-110	Purification Tower 2 Condenser	Fabricated Equipment
P-101	Recycle Water Pump	Process Machinery
P-102	Purification Tower 1 Reflux Pump	Process Machinery
P-103	Purification Tower 2 Reflux Pump	Process Machinery
R-101	Microchannel Reactor system	Fabricated Equipment
CO2SCRUB	MEA CO2 Scrubbing Unit based on GTL	Fabricated Equipment

8.1.2 Block 200

Equipment Number	Name	Type
H-204	Distillation Column D – 201 Condenser	Fabricated Equipment
H-205	Distillation Column D – 201 Reboiler	Fabricated Equipment
H-206	Distillation Column D – 202 Condenser	Fabricated Equipment
H-207	Distillation Column D – 202 Reboiler	Fabricated Equipment
H-208	Distillation Column D – 203 Condenser	Fabricated Equipment
H-209	Distillation Column D – 203 Reboiler	Fabricated Equipment
F-201	CO Purge vessel	Fabricated Equipment
F-202	EO and CO purge vessel	Fabricated Equipment
H-203	Ethylene Oxide Heater	Fabricated Equipment
H-202	β-propiolactone cooler	Fabricated Equipment
H-203	β-propiolactone condenser	Fabricated Equipment
K-201	Distillation Column 3 feed compressor	Process Machinery
D-201	Distillation Column 1	Fabricated Equipment
D-202	Distillation Column 2	Fabricated Equipment
D-203	Distillation Column 3	Fabricated Equipment
R-201	CSTR Reactor 1	Fabricated Equipment
R-202	CSTR Reactor 2	Fabricated Equipment
R-203	CSTR Reactor 3	Fabricated Equipment
V-201	Distillation Column 1 Vacuum	Fabricated Equipment
V-202	Distillation Column 2 Vacuum	Fabricated Equipment
P-201	Distillation Column D-201 reflux pump	Process Machinery
P-202	Distillation Column D-202 reflux pump	Process Machinery
P-203	Distillation Column D-203 reflux pump	Process Machinery
C-201	Condenser Accumulator D-201	Fabricated Equipment
C-202	Condenser Accumulator D-202	Fabricated Equipment
C-203	Condenser Accumulator D-203	Fabricated Equipment

8.1.3 Block 300

Equipment Number	Name	Type
F-302	Flash purification of Acrylic Acid Product	Fabricated Equipment
H-301	Reactor outlet condenser	Fabricated Equipment
H-302	Acrylic Acid Condenser	Fabricated Equipment
P-301	Feed pump for D-301	Process Machinery
P-302	Storage Pump	Process Machinery
C-301	Reflux Accumulator for D-301	Fabricated Equipment
H-303	Condenser for D-301	Fabricated Equipment
K-301	Reboiler for D-301	Fabricated Equipment
R-301	β-Propiolactone to Acrylic Acid Reactor	Fabricated Equipment
D-301	Distillation Tower for Acrylic Acid	Fabricated Equipment
P-303	Reflux Pump for D-301	Process Machinery
V-301	Reactor Vacuum	Fabricated Equipment
F-303	Flash to Vacuum System	Fabricated Equipment
ST-301	Acrylic Acid storage tank	Fabricated Equipment

8.2 Unit Specification Sheets

8.2.1 Pumps

P – 101				
Identification	**Equipment**	Pump		
	Inlet Stream	S – 123		
	Outlet Stream	S - 124		
Function	Water recycle pump for ethylene oxide absorber			
Type	Centrifugal Pump 3600 RPM, VSC, 300 - 1100 ft, 50 – 1100 gpm, 250 Hp			
Design	**Efficiency** (%)	66	**Inlet Pressure** (psia)	15
	Casing Material	Stainless Steel	**Outlet Pressure** (psia)	334
	Fluid Head (ft)	750	**Net Work** (Hp)	3.54
	Liquid Flow Rate (GPM)	321	**Electricity** (kW)	
	Installed Weight (lbs)	10,626		
Cost	**Purchase** (USD)	5,070	**Bare Module** (USD)	39,025

P – 102				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for column D - 103			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	70	**Inlet Pressure** (psia)	
	Casing Material	Stainless Steel	**Outlet Pressure** (psia)	
	Fluid Head (ft)	200	**Net Work** (Hp)	
	Liquid Flow Rate (GPM)	473.7	**Electricity** (kW)	
	Installed Weight (lbs)	8430		
Cost	**Purchase** (USD)	4,640	**Bare Module** (USD)	19,953

P – 103				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for Column D-104			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	70	**Inlet Pressure** (psia)	
	Casing Material	Stainless Steel	**Outlet Pressure** (psia)	
	Fluid Head (ft)	200	**Net Work** (Hp)	
	Liquid Flow Rate (GPM)	77	**Electricity** (kW)	
	Installed Weight (lbs)	3103		
Cost	**Purchase** (USD)	3,120	**Bare Module** (USD)	13,420

P – 201				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for the Distillation Column D-201			
Type	Centrifugal Pump 3600 RPM, HSC, 100 - 450 ft, 100 - 1500 gpm, 150 Hp			
Design	**Efficiency** (%)	100	**Inlet Pressure** (psia)	25.053
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	107.203
	Fluid Head (ft)	100	**Net Work** (Hp)	3.54
	Liquid Flow Rate (GPM)	1223.75	**Electricity** (kW)	2.64
	Installed Weight (lbs)	4270		
Cost	**Purchase** (USD)	5,708.52	**Bare Module** (USD)	22,834.08

P – 202				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for the Distillation Column D-202			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	100	**Inlet Pressure** (psia)	23.353
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	105.503
	Fluid Head (ft)	35	**Net Work** (Hp)	2.22
	Liquid Flow Rate (GPM)	150	**Electricity** (kW)	1.655
	Installed Weight (lbs)	4240		
Cost	**Purchase** (USD)	3,049.79	**Bare Module** (USD)	10,064.31

P – 203				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for the Distillation Column D-203			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	100	**Inlet Pressure** (psia)	36.053
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	118.203
	Fluid Head (ft)	25.5	**Net Work** (Hp)	2
	Liquid Flow Rate (GPM)	45	**Electricity** (kW)	1
	Installed Weight (lbs)	5210		
Cost	**Purchase** (USD)	2,964.23	**Bare Module** (USD)	9,781.97

P – 301				
Identification	**Equipment**	Pump		
	Inlet Stream	S – 312		
	Outlet Stream	S - 313		
Function	Increase pressure before going into Distillation Column			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	50	**Inlet Pressure** (psia)	1.83
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	40.75
	Fluid Head (ft)	78.46	**Net Work** (Hp)	3.54
	Liquid Flow Rate (GPM)	90.95	**Electricity** (kW)	2.64
	Installed Weight (lbs)	4270		
Cost	**Purchase** (USD)	2,983	**Bare Module** (USD)	9,900

P – 302				
Identification	**Equipment**	Pump		
	Inlet Stream	S - 323		
	Outlet Stream	S - 324		
Function	Increase pressure in the Final Product Stream			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	70	**Inlet Pressure** (psia)	15
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	50
	Fluid Head (ft)	78.36	**Net Work** (Hp)	2.22
	Liquid Flow Rate (GPM)	79.54	**Electricity** (kW)	1.655
	Installed Weight (lbs)	4240		
Cost	**Purchase** (USD)	2,983	**Bare Module** (USD)	9,844

P – 303				
Identification	**Equipment**	Pump		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Reflux Pump for the Distillation Column			
Type	Centrifugal Pump 3600 RPM, VSC, 40-500 ft, 40 – 900 gpm, 75 Hp			
Design	**Efficiency** (%)	100	**Inlet Pressure** (psia)	40.75
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	50
	Fluid Head (ft)	98.65	**Net Work** (Hp)	2
	Liquid Flow Rate (GPM)	42	**Electricity** (kW)	1
	Installed Weight (lbs)	5210		
Cost	**Purchase** (USD)	2,965	**Bare Module** (USD)	9,780

8.2.2 Heat Exchangers

H - 101				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S-103	**Temperature** (F)	71.4
	Outlet Stream	S-104	**Temperature (**F)	482
Function	Inlet Gas heater to achieve Reactor conditions at 300PSIA and 250ºC			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	1700		
	Tube Temperature (F)	482	**Tube Material**	Stainless Steel
	Shell Temperature (F)	600	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	37,400		
Cost	**Purchase** (USD)	21,400	**Bare Module** (USD)	115,00

H - 102				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S-107	**Temperature** (F)	425
	Outlet Stream	S-108	**Temperature (**F)	94
Function	Outlet gas cooler and condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	3000		
	Tube Temperature (F)	95	**Tube Material**	Carbon Steel
	Shell Temperature (F)	425	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	57,000		
Cost	**Purchase** (USD)	35,100	**Bare Module** (USD)	200,590

H -103				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S-113	**Temperature** (F)	280
	Outlet Stream	S-114	**Temperature (**F)	-28
Function	Purification tower 2 inlet stream condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	7,470		
	Tube Temperature (F)	-40	**Tube Material**	Stainless Steel
	Shell Temperature (F)	280	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	87,200		
Cost	**Purchase** (USD)	58,680	**Bare Module** (USD)	335,615

H – 104				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	120	**Temperature** (F)	233
	Outlet Stream	123	**Temperature (**F)	90
Function	Recycle water condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	6,900		
	Tube Temperature (F)	95	**Tube Material**	Stainless Steel
	Shell Temperature (F)	233	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	77,280		
Cost	**Purchase** (USD)	54,960	**Bare Module** (USD)	310,750

H – 105				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 122	**Temperature** (F)	233
	Outlet Stream	S – 106	**Temperature (**F)	1
Function	Quench steam heater			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	940		
	Tube Temperature (F)		**Tube Material**	Stainless Steel
	Shell Temperature (F)		**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)			
Cost	**Purchase** (USD)	16,000	**Bare Module** (USD)	86,690

H - 106				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	280
	Outlet Stream	-	**Temperature (**F)	350
Function	Reboiler for D-102			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	42720		
	Tube Temperature (F)	363.6	**Tube Material**	Stainless Steel
	Shell Temperature (F)	357.867205	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	418,352		
Cost	**Purchase** (USD)	343,830	**Bare Module** (USD)	2,124,185

H - 107				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	186.7
	Outlet Stream	-	**Temperature (**F)	186.7
Function	Reboiler for D-103			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	5606		
	Tube Temperature (F)	327.8	**Tube Material**	Stainless Steel
	Shell Temperature (F)	192	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	72,818		
Cost	**Purchase** (USD)	46,640	**Bare Module** (USD)	263,450

H - 108				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	220.4
	Outlet Stream	-	**Temperature (**F)	220.4
Function	Reboiler for D-104			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	686		
	Tube Temperature (F)	327.8	**Tube Material**	Stainless Steel
	Shell Temperature (F)	232	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	20,290		
Cost	**Purchase** (USD)	14,210	**Bare Module** (USD)	73,963

H - 109				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	3.6
	Outlet Stream	-	**Temperature (**F)	3.6
Function	Condenser for Column D-103			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	13,944		
	Tube Temperature (F)	-21.64	**Tube Material**	Stainless Steel
	Shell Temperature (F)	92	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	132,511		
Cost	**Purchase** (USD)	102,290	**Bare Module** (USD)	599,540

H - 110				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	65
	Outlet Stream	-	**Temperature (**F)	65
Function	Condenser for D-104			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	840		
	Tube Temperature (F)	-22	**Tube Material**	Stainless Steel
	Shell Temperature (F)	84	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	19,557		
Cost	**Purchase** (USD)	15,350	**Bare Module** (USD)	80,400

H - 201				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 216	**Temperature** (F)	236.322
	Outlet Stream	S – 217	**Temperature (**F)	213.345
Function	Condense beta-propiolactone into liquid			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	551.38094		
	Tube Temperature (F)	160	**Tube Material**	Stainless Steel
	Shell Temperature (F)	336	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	17247		
Cost	**Purchase** (USD)	24,500	**Bare Module** (USD)	77,700

H – 202				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 217	**Temperature** (F)	213.345
	Outlet Stream	S – 218	**Temperature (**F)	100.747
Function	Cool beta-propiolactone to 100 F			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	280.402		
	Tube Temperature (F)	95	**Tube Material**	Stainless Steel
	Shell Temperature (F)	213.344	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	14,500		
Cost	**Purchase** (USD)	10,138.94	**Bare Module** (USD)	60,274.41

H – 203				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 230	**Temperature** (F)	-4
	Outlet Stream	S – 231	**Temperature (**F)	176
Function	Heat ethylene oxide to 80 C and 600 psig with heat from sulfolane			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	5.526		
	Tube Temperature (F)	465.461	**Tube Material**	Stainless Steel
	Shell Temperature (F)	176	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	4599		
Cost	**Purchase** (USD)	9,364.06	**Bare Module** (USD)	62,463.49

H – 204				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 220	**Temperature** (F)	464.522
	Outlet Stream	S – 221	**Temperature (**F)	176
Function	Heating sulfolane			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	3344.01		
	Tube Temperature (F)	95	**Tube Material**	Stainless Steel
	Shell Temperature (F)	464.522	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	64167		
Cost	**Purchase** (USD)	29,670.68	**Bare Module** (USD)	206,862.26

H - 205				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-		
	Outlet Stream	-		
***Function**	Distillation Column (D – 201) Condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	18234		
	Tube Temperature (F)	-40	**Tube Material**	Stainless Steel
	Shell Temperature (F)	19.356	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	12669		
Cost	**Purchase** (USD)	9,809.54	**Bare Module** (USD)	58,173.38

H – 206				
Identification	**Equipment**	Heat Exchanger		
Function	Distillation Column (D – 201) Reboiler			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	7911.61		
	Tube Temperature (F)	449.704	**Tube Material**	Stainless Steel
	Shell Temperature (F)	600	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	110084		
Cost	**Purchase** (USD)	57,215.94	**Bare Module** (USD)	356,337.10

H – 207				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Distillation Column (D – 202) Condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	859.781		
	Tube Temperature (F)	95	**Tube Material**	Stainless Steel
	Shell Temperature (F)	310.9943	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	19129		
Cost	**Purchase** (USD)	14,178.05	**Bare Module** (USD)	85,529.61

H – 208				
Identification	**Equipment**	Heat Exchanger		
Function	Distillation Column (D – 202) Reboiler			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	3966.880		
	Tube Temperature (F)	465.461	**Tube Material**	Stainless Steel
	Shell Temperature (F)	600	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	113690		
Cost	**Purchase** (USD)	33,407.51	**Bare Module** (USD)	205,919.64

H – 209				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-		
	Outlet Stream	-		
Function	Distillation Column (D – 203) Condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	599.843		
	Tube Temperature (F)	-21.64	**Tube Material**	Stainless Steel
	Shell Temperature (F)	53.343	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	18324		
Cost	**Purchase** (USD)	12,390.88	**Bare Module** (USD)	74,389.97

H – 210				
Identification	**Equipment**	Heat Exchanger		
Function	Distillation Column (D – 203) Reboiler			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	163.168		
	Tube Temperature (F)	327.8	**Tube Material**	Stainless Steel
	Shell Temperature (F)	92.873	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	7746		
Cost	**Purchase** (USD)	9,422.31	**Bare Module** (USD)	55,637.48

H – 211				
Identification	**Equipment**	Heat Exchanger		
Function	Reactor (R-201) Heat Exchanger			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	618.15		
	Tube Temperature (F)	77	**Tube Material**	Stainless Steel
	Shell Temperature (F)	176	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	-		
Cost	**Purchase** (USD)	22,640.20	**Bare Module** (USD)	149,454.10

H – 212				
Identification	**Equipment**	Heat Exchanger		
Function	Reactor (R-201) Heat Exchanger			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	618.15		
	Tube Temperature (F)	77	**Tube Material**	Stainless Steel
	Shell Temperature (F)	176	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	-		
Cost	**Purchase** (USD)	22,640.20	**Bare Module** (USD)	149,454.10

H – 213				
Identification	**Equipment**	Heat Exchanger		
Function	Reactor (R-201) Heat Exchanger			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	618.15		
	Tube Temperature (F)	77	**Tube Material**	Stainless Steel
	Shell Temperature (F)	176	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	-		
Cost	**Purchase** (USD)	22,640.20	**Bare Module** (USD)	149,454.10

H - 301				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 307	**Temperature** (F)	337
	Outlet Stream	S – 310	**Temperature** (F)	175
Function	Condense acrylic acid after the reaction zone			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	795		
	Tube Temperature (F)	160	**Tube Material**	Carbon Steel
	Shell Temperature (F)	336	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	21,450		
Cost	**Purchase** (USD)	24,500	**Bare Module** (USD)	77,700

H - 302				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S – 314	**Temperature** (F)	346
	Outlet Stream	S – 320	**Temperature** (F)	100
Function	Condense acrylic acid after the distillation column			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	470		
	Tube Temperature (F)	160	**Tube Material**	Carbon Steel
	Shell Temperature (F)	346	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	14,500		
Cost	**Purchase** (USD)	11,500	**Bare Module** (USD)	36,400

H - 303				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	-	**Temperature** (F)	
	Outlet Stream	-	**Temperature (**F)	
Function	Distillation Column (D – 301) Condenser			
Type	Shell and Tube			
Design	**Exchange Area** (ft^2)	230		
	Tube Temperature (F)	95	**Tube Material**	Carbon Steel
	Shell Temperature (F)	350	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	10,890		
Cost	**Purchase** (USD)	18,600	**Bare Module** (USD)	59,000

H – 304				
Identification	**Equipment**	Heat Exchanger		
Function	Reboiler in Distillation Column D-301			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	2400		
	Tube Temperature (F)	445	**Tube Material**	Carbon Steel
	Shell Temperature (F)	387	**Shell Material**	Carbon Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	40,711		
Cost	**Purchase** (USD)	26,065	**Bare Module** (USD)	145,460

H – 305				
Identification	**Equipment**	Heat Exchanger		
Function	Reactor (R-301) Heat Exchanger			
Type	Kettle Reboiler			
Design	**Exchange Area** (ft^2)	200.96		
	Tube Temperature (F)	459.565	**Tube Material**	Stainless Steel
	Shell Temperature (F)	338	**Shell Material**	Stainless Steel
	Tube Pitch (inches)	1.25	**Tube Length** (ft)	20
	Installed Weight (lbs)	-		
Cost	**Purchase** (USD)	18,383.25	**Bare Module** (USD)	108,830.09

8.2.3 Flash Vessels

F – 201				
Identification	**Equipment**	Flash Vessel		
	Inlet Stream	S-229		
	Overhead	S-237		
	Bottoms	S-230		
Function	Purges CO			
Design	**Temperature (F)**	176	**Construction Material**	Stainless Steel 316
	Light Flow Rate (lb/hr)	-	**Heavy Flow Rate (lb/hr)**	37,360
	Liquid Volume (gal)	1175	**Pressure (psia)**	614.7
	Tangent Height (ft)	12	**Diameter (ft)**	3
	Installed Weight (lbs)	6470	**Vessel Wall Thickness (in)**	1.132
Cost	**Purchase** (USD)	72,615.00	**Bare Module** (USD)	302,078.40

F – 202				
Identification	**Equipment**	Flash Vessel		
	Inlet Stream	S-231		
	Overhead	S-238		
	Bottoms	S-232		
Function	Purges evaporated EO and CO			
Design	**Temperature (F)**	176	**Construction Material**	Stainless Steel 316
	Light Flow Rate (lb/hr)	-	**Heavy Flow Rate (lb/hr)**	37,360
	Liquid Volume (gal)	1175	**Pressure (psia)**	614.7
	Tangent Height (ft)	12	**Diameter (ft)**	3
	Installed Weight (lbs)	6470	**Vessel Wall Thickness (in)**	1.132
Cost	**Purchase** (USD)	72,615.00	**Bare Module** (USD)	302,078.40

F – 301				
Identification	**Equipment**	Flash Vessel		
	Inlet Stream	S-318, S-320, S-319		
	Overhead	S-321		
	Bottoms	S-323		
Function	Allows Nitrogen purge			
Design	**Temperature (F)**	100	**Construction Material**	Carbon Steel
	Light Flow Rate (lb/hr)	-	**Heavy Flow Rate (lb/hr)**	37,360
	Liquid Volume (gal)	1175	**Pressure (psia)**	15
	Tangent Height (ft)	12.5	**Diameter (ft)**	4
	Installed Weight (lbs)	14,570		
Cost	**Purchase** (USD)	15,880	**Bare Module** (USD)	48,430

8.2.4 Columns

D – 101				
Identification	**Equipment**	Absorber		
Function	EO Absorber			
Design	**Number of Trays**	10	**Tray Spacing** (ft)	2
	Total Weight (lbs)	63,367	**Tray Type**	Valve
	Feed Stage	-	**Tray Efficiency** (%)	0.7
	Total Height (ft)	42	**Condenser Type**	-
	Construction Material	Stainless Steel 304	**Condenser Duty** (Btu/hr)	-
	Reboiler Pressure (psia)	-	**Reboiler Duty** (Btu/hr)	-
	Condenser Pressure (psia)	-	**Reflux Ratio**	-
	Column Diameter (ft)	6		
Materials	**Feed**	**Absorbent**	**Scrubbed Gas**	**Bottoms**
Stream ID	S-108	S-109	S-111	S-110
Temperature (F)	94	92	92	110.4
Pressure (psia)	215	334	200	201
Total Flow Rate (lb/hr)	159818	144303	60508.38	243613
Component Flow Rates (lb/hr)				
Ethylene	68700	9	25944	42766
Oxygen	20373	0.003	18956	1418
Ethylene Oxide	24412	71	10	24474
Formaldehyde	4588	113	9	4692
Acetaldehyde	67.5	0.4	0.03	69
Carbon Dioxide	7282	0.4	2625	4658
Water	20181	144110	84	164207
Argon	9123	0.001	8511	612
Methane	5090	0.008	4371	719
Cost	**Purchase** (USD)	205,335	**Bare Module** (USD)	854,194

D – 102				
Identification	**Equipment**			
Function	EO Stripping Column			
Design	**Number of Trays**	2	**Tray Spacing** (ft)	2
	Total Weight (lbs)	54660	**Tray Type**	Valve
	Feed Stage	1	**Tray Efficiency** (%)	0.7
	Total Height (ft)	42	**Condenser Type**	-
	Construction Material	Stainless Steel 304	**Condenser Duty** (Btu/hr)	-
	Reboiler Pressure (psia)	150.3	**Reboiler Duty** (Btu/hr)	$7.4*10^7$
	Condenser Pressure (psia)	-	**Reflux Ratio**	-
	Column Diameter (ft)	6		
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-110		S-113	S-112
Temperature (F)	110.3913		279.6362	357.8672
Pressure (psia)	200.9		150	150.3
Total Flow Rate (lb/hr)	243613		99402.03	144211
Component Flow Rates (lb/hr)				
Ethylene	42766		42755.74	10
Oxygen	1418		1417.655	0.004
Ethylene Oxide	24475		24416.99	57
Formaldehyde	4692		4564.452	128
Acetaldehyde	68		67.87386	0.01
Carbon Dioxide	4658		4657.249	0.51
Water	164207		20191.06	144016
Argon	612		612.0002	0.001
Methane	719		719.002	0.01
Cost	**Purchase** (USD)	121,905	**Bare Module** (USD)	507,127

D – 103				
Identification	**Equipment**			
Function	EO Purification Tower 1			
Design	**Number of Trays**	40	**Tray Spacing** (ft)	2
	Total Weight (lbs)	350220	**Tray Type**	Valve
	Feed Stage	10	**Tray Efficiency** (%)	0.7
	Total Height (ft)	92	**Condenser Type**	Partial Vapor
	Construction Material	Stainless Steel 304	**Condenser Duty** (Btu/hr)	$-6.7*10^7$
	Reboiler Pressure (psia)	142.9	**Reboiler Duty** (Btu/hr)	$8.3*10^7$
	Condenser Pressure (psia)	140	**Reflux Ratio**	3.94
	Column Diameter (ft)	12		
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-114		S-116	S-115
Temperature (F)	-29		3.6	191.5
Pressure (psia)	145		140	142.9
Total Flow Rate (lb/hr)	99402		54802	44600
Component Flow Rates (lb/hr)				
Ethylene	42756		42756	0
Oxygen	1418		1418	0
Ethylene Oxide	24417		122	24295
Formaldehyde	4564		4519	45.6
Acetaldehyde	68		0.00	68
Carbon Dioxide	4657		4657	0
Water	20191		0	20191
Argon	612		612	0
Methane	719		719	0
Cost	**Purchase** (USD)	959,172	**Bare Module** (USD)	3,990,157

D – 104				
Identification	**Equipment**			
Function	EO Purification Tower 2			
Design	**Number of Trays**	13	**Tray Spacing** (ft)	2
	Total Weight (lbs)	56420	**Tray Type**	Valve
	Feed Stage	11	**Tray Efficiency** (%)	0.7
	Total Height (ft)	50	**Condenser Type**	Partial Vapor
	Construction Material	Stainless Steel 304	**Condenser Duty** (Btu/hr)	$-8.9*10^6$
	Reboiler Pressure (psia)	22.1	**Reboiler Duty** (Btu/hr)	$1.34*10^7$
	Condenser Pressure (psia)	20	**Reflux Ratio**	1.44
	Column Diameter (ft)	5		
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-115		S-118	S-117
Temperature (F)	191		65	232
Pressure (psia)	1423		20	22.1
Total Flow Rate (lb/hr)	44600		24393	20206
Component Flow Rates (lb/hr)				
Ethylene Oxide	24295		24270.61	24.3
Formaldehyde	46		44.92382	0.72
Acetaldehyde	68		67.41851	0.45
Water	20191		10.0956	20181
Cost	**Purchase** (USD)	149,800	**Bare Module** (USD)	623,185

D – 201				
Identification	**Equipment**	Distillation Column		
Function	Separate ethylene oxide, CO, and acetaldehyde to the distillate			
Design	**Number of Trays**	20	**Tray Spacing** (ft)	1.5
	Total Weight (lbs)	8462	**Tray Type**	Koch Flexitray
	Feed Stage	7	**Tray Efficiency**	0.7
	Total Height (ft)	33	**Condenser Type**	Partial - Vapor
	Construction Material	Stainless Steel 316	**Condenser Duty** (Btu/hr)	-7,700,000
	Reboiler Pressure (psia)	42.1	**Reboiler Duty** (Btu/hr)	16,000,000
	Condenser Pressure (psia)	38	**Reflux Ratio**	1.2
	Diameter (ft)	Refer to unit descriptions	**Wall Thickness** (in)	0.438
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-213		S-214	S-215
Temperature (F)	176		-12.69	449.705
Pressure (psia)	614.7		3.7	6.85
Total Flow Rate (lb/hr)	727240		9113.38	715126
Component Flow Rates (lb/hr)				
CO	235.8447		189.6049	8.77E-24
BETA--01	0		0.010158	519.5091
ETHYL-01	179.2796		56.10447	8.13E-10
SULFO-01	0		1.09E-34	5639.308
ACETA-01	1.792796		30.19443	3.06E-09
Cost	**Purchase** (USD)	1,040,926	**Bare Module** (USD)	4,330,202

D – 202				
Identification	**Equipment**	Distillation Column		
Function	Separate beta-propiolactone to the distillate, sulfolane and catalyst to the bottoms			
Design	**Number of Trays**	9	**Tray Spacing** (ft)	2
	Total Weight (lbs)	21256	**Tray Type**	Koch Flexitray
	Feed Stage	7	**Tray Efficiency**	0.7
	Total Height (ft)	22	**Condenser Type**	Partial - Vapor
	Construction Material	Stainless Steel 316	**Condenser Duty** (Btu/hr)	-7,700,000
	Reboiler Pressure (psia)	42.1	**Reboiler Duty** (Btu/hr)	16,000,000
	Condenser Pressure (psia)	38	**Reflux Ratio**	1.8
	Diameter (ft)	9.820	**Wall Thickness** (in)	0.563
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-215		S-216	S-219
Temperature (F)	449.705		236.323	465.461
Pressure (psia)	6.85		2	3.5
Total Flow Rate (lb/hr)	715126		37485.62	677641
Component Flow Rates (lb/hr)				
Nitrogen	8.77E-24		0	0
Beta-Lactone	519.5091		518.5248	0.984273
Phosphoric Acid	8.13E-10		8.13E-10	2.35E-23
Water	5639.308		0.989211	5638.318
Acrylic Acid	3.06E-09		3.06E-09	3.96E-22
Cost	**Purchase** (USD)	113,660	**Bare Module** (USD)	472,840

D – 203				
Identification	**Equipment**	Distillation Column		
Function	Separate ethylene oxide and CO from acetaldehyde, acetaldehyde is purged through bottoms			
Design	**Number of Trays**	10	**Tray Spacing** (ft)	2
	Total Weight (lbs)	4024	**Tray Type**	Koch Flexitray
	Feed Stage	7	**Tray Efficiency**	0.7
	Total Height (ft)	24	**Condenser Type**	Partial - Vapor
	Construction Material	Stainless Steel 316	**Condenser Duty** (Btu/hr)	-7,700,000
	Reboiler Pressure (psia)	42.1	**Reboiler Duty** (Btu/hr)	16,000,000
	Condenser Pressure (psia)	38	**Reflux Ratio**	1.8
	Diameter (ft)	3.126	**Wall Thickness** (in)	0.3756
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-228		S-229	S-236
Temperature (F)	-30.42		12.7627	92.893
Pressure (psia)	17		14.7	16.95
Total Flow Rate (lb/hr)	9113.382		8147.716	965.6655
Component Flow Rates (lb/hr)				
Nitrogen	189.6049		189.6049	1.79E-24
Beta-Lactone	0.010158		1.02E-28	0.010158
Phosphoric Acid	56.10447		54.59004	1.51443
Water	1.09E-34		0	0
Acrylic Acid	30.19443		9.805019	20.38941
Cost	**Purchase** (USD)	102,719.59	**Bare Module** (USD)	427,313.50

D – 301				
Identification	**Equipment**	Distillation Column		
Function	Separate acrylic acid product			
Design	**Number of Trays**	16	**Tray Spacing** (ft)	2
	Total Weight (lbs)	11,400	**Tray Type**	Valve
	Feed Stage	7	**Tray Efficiency** (%)	70
	Total Height (ft)	42	**Condenser Type**	Partial - Vapor
	Construction Material	Carbon Steel	**Condenser Duty** (Btu/hr)	-7,700,000
	Reboiler Pressure (psia)	42.1	**Reboiler Duty** (Btu/hr)	16,000,000
	Condenser Pressure (psia)	38	**Reflux Ratio**	1.2
	Diameter (ft)	5.5		
Materials	**Feed**	**Liquid Distillate**	**Vapor Distillate**	**Bottoms**
Stream ID	S-313		S-314	S-315
Temperature (F)	175		346	386
Pressure (psia)	40.75		38	42
Total Flow Rate (lb/hr)	38,780		37,330	1450
Component Flow Rates (lb/hr)				
Nitrogen	0		0	0
Beta-Lactone	15.8		2.5	13.5
Phosphoric Acid	0		0	0
Water	0.9		0.9	0
Acrylic Acid	521		515	5.2
MEHQ	1		0	1
Cost	**Purchase** (USD)	113,660	**Bare Module** (USD)	472,840

8.2.5 Reactors

R – 101				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-104		
	Outlet Stream	S-105		
Main Reaction	Ethylene + O_2 -> Ethylene Oxide			
Side Reactions	Ethylene + O_2 -> CO_2, Water, Acetaldehyde, Formaldehyde			
Classification	Microchannel Reactor			
Design	**Temperature** (F)	482	**Construction Material**	Stainless Steel 304
	Pressure (Psia)	290	**Heat Duty** (W)	27000
	Diameter (ft)	-	**Residence Time** (s)	0.5
	Tangent Height (ft)	-	**Vessel Weight** (tonne)	9600
	Electricity (kW)	-		
	Volume (ft^3)	8551.757		
Cost	**Purchase of Vessel** (USD)	27M	**Total Bare Module**	135M

R – 201				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-201, S-202, S-203		
	Outlet Stream	S-210		
Main Reaction	CO + Ethylene oxide -> Beta-propiolactone			
Side Reactions	Ethylene Oxide -> Acetaldehyde, CO + Beta-propiolactone -> Succinic anhydride			
Classification	CSTR			
Design	**Temperature** (F)	176	**Construction Material**	Stainless Steel 316
	Pressure (Psia)	614.7	**Heat Duty** (Btu/hr)	$1.3*10^6$
	Diameter (ft)	7.395	**Residence Time** (hr)	0.198
	Tangent Height (ft)	26.621	**Vessel Weight** (lbs)	70269
	Electricity (kW)			
	Volume (gal)	8551.757		
Cost	**Purchase of Vessel** (USD)	92,600	**Bare Module of Vessel** (USD)	282,425
	Cost of Agitator (USD)	3,768.79	**Total Bare Module**	286,193.79

R – 202				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-204, S-205, S-206		
	Outlet Stream	S-211		
Main Reaction	CO + Ethylene oxide -> Beta-propiolactone			
Side Reactions	Ethylene Oxide -> Acetaldehyde, CO + Beta-propiolactone -> Succinic anhydride			
Classification	CSTR			
Design	**Temperature** (F)	176	**Construction Material**	Stainless Steel 316
	Pressure (Psia)	614.7	**Heat Duty** (Btu/hr)	$1.3*10^6$
	Diameter (ft)	7.395	**Residence Time** (hr)	0.198
	Tangent Height (ft)	26.621	**Vessel Weight** (lbs)	70269
	Electricity (kW)			
	Volume (gal)	8551.757		
Cost	**Purchase** (USD)	92,600	**Bare Module** (USD)	282,425
	Cost of Agitator (USD)	3,768.79	**Total Bare Module**	286,193.79

R – 203				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-207, S-208, S-209		
	Outlet Stream	S-212		
Main Reaction	CO + Ethylene oxide -> Beta-propiolactone			
Side Reactions	Ethylene Oxide -> Acetaldehyde, CO + Beta-propiolactone -> Succinic anhydride			
Classification	CSTR			
Design	**Temperature** (F)	176	**Construction Material**	Stainless Steel 316
	Pressure (Psia)	614.7	**Heat Duty** (Btu/hr)	$1.3*10^6$
	Diameter (ft)	7.395	**Residence Time** (hr)	0.198
	Tangent Height (ft)	26.621	**Vessel Weight** (lbs)	70269
	Electricity (kW)			
	Volume (gal)	8551.757		
Cost	**Purchase** (USD)	92,600	**Bare Module** (USD)	282,425
	Cost of Agitator (USD)	3,768.79	**Total Bare Module**	286,193.79

R – 301				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-301, S-302, S-315		
	Outlet Stream	S-303		
Main Reaction	$C_3H_4O_2 \rightarrow C_3H_4O_2$			
Side Reactions	$C_3H_4O_2 \rightarrow (C_3H_4O_2)_n$			
Classification	Stirred Tank Reactor			
Design	**Temperature** (F)	338	**Construction Material**	Hastelloy C
	Pressure (Psia)	1.93	**Heat Duty** (Btu/hr)	$1.3*10^6$
	Diameter (ft)	8	**Residence Time** (hr)	2.8
	Tangent Height (ft)	8	**Vessel Weight** (lbs)	7428
	Electricity (kW)			
	Volume (gal)	11,710		
Cost	**Purchase** (USD)	92,600	**Bare Module** (USD)	282,425

8.2.6 Condenser Accumulators

C – 101				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-103			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	3021	**Construction Material**	Stainless Steel 304
	Diameter (ft)	5.5	**Temperature** (F)	3.6
	Tangent Height (ft)	17	**Installed Weight** (lbs)	22031
Cost	**Purchase** (USD)	58,175	**Bare Module** (USD)	177,432

C – 102				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-104			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	500	**Construction Material**	Stainless Steel 304
	Diameter (ft)	3	**Temperature** (F)	32
	Tangent Height (ft)	8.5	**Installed Weight** (lbs)	7582
Cost	**Purchase** (USD)	27,405	**Bare Module** (USD)	83,600

C – 201				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-201			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	476	**Construction Material**	Stainless Steel 316
	Diameter (ft)	3	**Temperature** (F)	-22.76
	Tangent Height (ft)	9	**Installed Weight** (lbs)	1662
Cost	**Purchase** (USD)	33,832.49	**Bare Module** (USD)	103,189.11

C – 202				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-202			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	1081.1	**Construction Material**	Stainless Steel 316
	Diameter (ft)	4	**Temperature** (F)	236
	Tangent Height (ft)	11.5	**Installed Weight** (lbs)	2851
Cost	**Purchase** (USD)	42,224.58	**Bare Module** (USD)	128,784.97

C – 203				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-203			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	476	**Construction Material**	Stainless Steel 316
	Diameter (ft)	3	**Temperature** (F)	12.76
	Tangent Height (ft)	9	**Installed Weight** (lbs)	2851
Cost	**Purchase** (USD)	33,832.49	**Bare Module** (USD)	103,189.11

C – 301				
Identification	**Equipment**	Condenser Accumulator		
Function	Condenser accumulator for distillation column D-301			
Classification	Horizontal Vessel			
Design	**Storage Volume** (gal)	720	**Construction Material**	Carbon Steel
	Diameter (ft)	3.5	**Temperature** (F)	346
	Tangent Height (ft)	10	**Installed Weight** (lbs)	
Cost	**Purchase** (USD)	19,290	**Bare Module** (USD)	58,830

8.2.7 Storage Tanks

ST - 301				
Identification	**Equipment**	Storage Tank		
	Inlet Stream	S-324		
Function	Acrylic Acid Storage			
Classification	Open Cone Storage Tank			
Design	**Storage Volume** (gal)	231,900	**Construction Material**	Stainless Steel
	Pressure (psia)	50	**Temperature** (F)	77
	Heat Duty (Btu/hr)			
Cost	**Purchase** (USD)	557,550	**Bare Module** (USD)	1,700,527

8.2.8 Vacuum Systems

V – 201				
Identification	**Equipment**	Vacuum		
	Unit Under Vacuum	D-201		
Function	Vacuum to maintain D-201 at 3.7 psia			
Classification	One-Stage Jet Ejector			
Design	**Leak Rate** (lb/hr)	227.523	**Construction Material**	Stainless Steel
	Flow of Vapor to Vacuum (lb/hr)	9113.38	**Size Factor**	48.815
	Total Flow to Vacuum (lb/hr)	9340.903		
Cost	**Purchase** (USD)	8,321.35	**Bare Module** (USD)	8,321.35

V – 202				
Identification	**Equipment**	Vacuum		
	Unit Under Vacuum	D-202		
Function	Vacuum to maintain D-202 at 2 psia			
Classification	One-Stage Jet Ejector			
Design	**Leak Rate** (lb/hr)	207.9404036	**Construction Material**	Stainless Steel
	Flow of Vapor to Vacuum (lb/hr)	37485.6	**Size Factor**	362.425
	Total Flow to Vacuum (lb/hr)	37693.54		
Cost	**Purchase** (USD)	18,930.67	**Bare Module** (USD)	18,930.67

V – 301				
Identification	**Equipment**	Vacuum		
	Inlet Stream	S-324		
Function	Maintain R-301 at a 1.93 psia			
Classification	Liquid Ring Pumps			
Design	**Leak Rate** (lb/hr)	16.2		
	Flow of Vapor to Vacuum (lb/hr)	20	**Size Factor** (ft^3/min)	10
	Total Flow to Vacuum (lb/hr)	36.2		
Cost	**Purchase** (USD)	18,470	**Bare Module** (USD)	18,470

8.2.9 Compressors

K – 201				
Identification	**Equipment**	Compressor		
Function	Increase vapor pressure before entering distillation column 3			
Classification	Centrifugal			
Design	**Gas Flow Inlet** (CFM)	5827.33	**Construction Material**	Stainless Steel
	Inlet Pressure (psia)	3.7	**Outlet Pressure** (psia)	17
	Tangent Height (ft)	10	**Installed Weight** (lbs)	46905
	Motor Power (Hp)	256.945		
Cost	**Purchase** (USD)	165,851.57	**Bare Module** (USD)	605,504.22

8.3 Unit Descriptions

8.3.1 Pumps

<u>P – 101</u>

Pump 101 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the recycle stream S-123, prior to feeding it into D-101 at a flow rate of 321 GPM as S-124. Its net work is 3.54 Hp and its installed weight is 10,626 lbs. Its purchase cost is $5,070 and the bare module cost is $39,025.

<u>P – 102</u>

Pump 102 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-103 at a flow rate of 473.7 GPM. Its installed weight is 8430 lbs. Its purchase cost is $4,640 and the bare module cost is $19,953.

<u>P – 103</u>

Pump 103 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-104 at a flow rate of 77 GPM. Its installed weight is 3103 lbs. Its purchase cost is $3,120 and the bare module cost is $13,420.

<u>P – 201</u>

Pump 201 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-201 at a flow rate of 1223.75 GPM. Its net work is 3.54 Hp, uses electricity of 2.64 kW, and its installed weight is 4270 lbs. Its purchase cost is $5,709 and the bare module cost is $22,834.

<u>P – 202</u>

Pump 202 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-202 at a flow rate of 150 GPM. Its net work is 2.22 Hp, uses electricity of 1.655 kW, and its installed weight is 4240 lbs. Its purchase cost is $3,049 and the bare module cost is $10,064.

<u>P – 203</u>

Pump 203 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-203 at a flow rate of 45 GPM. Its net work is 2 Hp, uses electricity of 1 kW, and its installed weight is 5210 lbs. Its purchase cost is $2,964 and the bare module cost is $9,782.

<u>P – 301</u>

Pump 301 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the stream S-312, prior to feeding it into D-301 at a flow rate of 90.95 GPM as S-313. Its net work is 3.54 Hp, uses electricity of 2.64 kW, and its installed weight is 4270 lbs. Its purchase cost is $2,983 and the bare module cost is $9,900.

<u>P – 302</u>

Pump 302 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the stream S-323, prior to feeding it into the product storage tank at a flow rate of 79.54 GPM as S-324. Its net work is 2.22 Hp, uses electricity of 1.655 kW, and its installed weight is 4270 lbs. Its purchase cost is $2,983 and the bare module cost is $9,844.

<u>P – 303</u>

Pump 303 is a cast iron 3600 RPM centrifugal pump used to increase the pressure of the reflux stream, prior to feeding it back into D-301 at a flow rate of 42 GPM. Its net work is 2 Hp, uses electricity of 1 kW, and its installed weight is 5210 lbs. Its purchase cost is $2,965 and the bare module cost is $9,780.

8.3.2 Heat Exchangers

<u>H – 101</u>

Heat Exchanger 101 is a single-pass shell and tube heat exchanger which receives stream S-103 at 71.4 degrees Fahrenheit and releases stream S-104 at 482 degrees Fahrenheit using steam. The tube is made of stainless steel, and the shell made of carbon steel. This allows the inlet gas to reach the reactor conditions at 300 psia and 250 degrees Celsius. The tube pitch is

1.25 inches, tube length 20 ft, effective heat transfer area 3,000 square feet, and its installed weight 57,000 lbs. The purchase and bare module costs are $35,100 and $200,590, respectively.

H – 102

Heat Exchanger 102 is a single-pass shell and tube heat exchanger which receives stream S-107 at 425 degrees Fahrenheit and releases stream S-108 at 95 degrees Fahrenheit using cooling water. The tube is made of carbon steel, and the shell made of stainless steel. The heat exchanger cools and condenses the outlet gas from the mix of S-105 and S-106. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 1700 square feet, and its installed weight 37,400 lbs. The purchase and bare module costs are $21,400 and $115,000, respectively.

H – 103

Heat Exchanger 103 is a single-pass shell and tube heat exchanger which receives stream S-113 at 280 degrees Fahrenheit and releases stream S-114 at -28 degrees Fahrenheit using refrigerant. The tube is made of stainless steel, and the shell made of carbon steel. The heat exchanger cools S-113 before the stream enters D-103. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 7,470 square feet, and its installed weight 87,200 lbs. The purchase and bare module costs are $58,600 and $335,615, respectively.

H – 104

Heat Exchanger 104 is a single-pass shell and tube heat exchanger which receives stream S-120 at 425 degrees Fahrenheit and releases stream S-123 at 90 degrees Fahrenheit using cooling water. The tube is made of stainless steel, and the shell made of carbon steel. The heat exchanger cools and condenses the stream before it enters the pump P-101. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 6,900 square feet, and its installed weight 77,280 lbs. The purchase and bare module costs are $54,960 and $310,750, respectively.

H – 105

Heat Exchanger 105 is a single-pass shell and tube heat exchanger which receives stream S-122 at 233 degrees Fahrenheit and releases stream S-106 at 1 degree Fahrenheit using steam. The tube is made of stainless steel, and the shell made of carbon steel. This heat exchanger functions as a quench steam heater. The tube pitch is 1.25 inches, tube length 20 ft, and effective heat transfer area 940 square feet. The purchase and bare module costs are $16,000 and $86,690, respectively.

H – 106

Heat Exchanger 106 is a single-pass shell and tube heat exchanger reboiler that boils and raises the temperature from 280 to 350 degrees Fahrenheit and releases the stream back into the distillation column using steam. The tube is made of stainless steel, and the shell made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 42,720 square feet, and installed weight 418,352 lbs. The purchase and bare module costs are $343,830 and $2,124,185, respectively.

H – 107

Heat Exchanger 107 is a single-pass shell and tube heat exchanger reboiler that boils the liquid and releases the stream back into the distillation column using steam. The tube is made of stainless steel, and the shell made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 5,606 square feet, and installed weight 72,818 lbs. The purchase and bare module costs are $46,640 and $263,450, respectively.

H – 108

Heat Exchanger 108 is a single-pass shell and tube heat exchanger reboiler that boils and raises the temperature from 220.4 degrees Fahrenheit and releases the stream back into the distillation column using steam. The tube is made of stainless steel, and the shell made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 42,720 square feet, and installed weight 20,290 lbs. The purchase and bare module costs are $14,210 and $73,963, respectively.

H – 109

Heat Exchanger 109 is a single-pass shell and tube heat exchanger condenser which condenses vapor and releases it back into the distillation column D-103 at 3.6 degrees Fahrenheit using refrigerant. The tube is made of stainless steel, and the shell made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 13,944 square feet, and its installed weight 132,511 lbs. The purchase and bare module costs are $102,290 and $599,540, respectively.

<u>H – 110</u>

Heat Exchanger 110 is a single-pass shell and tube heat exchanger condenser which condenses vapor and releases it back into the distillation column D-103 at 65 degrees Fahrenheit using refrigerant. The tube is made of stainless steel, and the shell made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 840 square feet, and its installed weight 19,557 lbs. The purchase and bare module costs are $15,350 and $80,400, respectively.

<u>H – 201</u>

Heat Exchanger 201 is a single-pass shell and tube heat exchanger which receives stream S-216 at 236.322 degrees Fahrenheit and releases stream S-218 at 213.345 degrees Fahrenheit using cooling water. The tube and shell are made of stainless steel. This heat exchanger condenses β-propiolactone into liquid. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 551.38 square feet, and its installed weight 17,247 lbs. The purchase and bare module costs are $12,051 and $72,267, respectively.

<u>H – 202</u>

Heat Exchanger 202 is a single-pass shell and tube heat exchanger which receives stream S-217 at 213.345 degrees Fahrenheit and releases stream S-218 at 100.747 degrees Fahrenheit using cooling water. The tube and shell are made of stainless steel. This heat exchanger further cools β-propiolactone stream. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 280.402 square feet, and its installed weight 14,500 lbs. The purchase and bare module costs are $10,139 and $60,274, respectively.

<u>H – 203</u>

Heat Exchanger 203 is a single-pass shell and tube heat exchanger which receives stream S-230 at -4 degrees Fahrenheit and releases stream S-231 at 176 degrees Fahrenheit using sulfolane. The tube and shell are made of stainless steel. This heat exchanger heats the recycled ethylene oxide to 80 degrees Celsius and 600 psig before it enters the reactor. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 5.526 square feet, and its installed weight 14,500 lbs. The purchase and bare module costs are $9,364.06 and $62,463, respectively. Because the heat exchanger price correlation uses a base cost that assumes that the price cannot be lower than what it is at the lowest surface area at 150 square feet, the price at 150 square feet was used.

H – 204

Heat Exchanger 204 is a single-pass shell and tube heat exchanger which receives stream S-220 at 464.522 degrees Fahrenheit and releases stream S-221 at 176 degrees Fahrenheit using cooling water. The tube and shell are made of stainless steel. This heat exchanger cools the sulfolane stream to 80 degrees Celsius and 600 psig before it enters the reactor. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 3344.01 square feet, and its installed weight 64167 lbs. The purchase and bare module costs are $29,671 and $206,862, respectively.

H – 205

Heat Exchanger 205 is a single-pass shell and tube heat exchanger condenser that condenses the vapor and releases the stream back into the distillation column D-201 using refrigerant. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 18,234 square feet, and installed weight 12,669 lbs. The purchase and bare module costs are $9,810 and $58,173, respectively.

H – 206

Heat Exchanger 206 is a single-pass shell and tube heat exchanger reboiler that boils the liquid and releases the stream back into the distillation column D-201 using steam. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 7,912 square feet, and installed weight 110,084 lbs. The purchase and bare module costs are $57,216 and $356,337, respectively.

H – 207

Heat Exchanger 207 is a single-pass shell and tube heat exchanger condenser that condenses the vapor and releases the stream back into the distillation column D-202 using refrigerant. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 860 square feet, and installed weight 19,129 lbs. The purchase and bare module costs are $14,178 and $85,530, respectively.

H – 208

Heat Exchanger 208 is a single-pass shell and tube heat exchanger reboiler that boils the liquid and releases the stream back into the distillation column D-202 using steam. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 3966.880 square feet, and installed weight 113,690 lbs. The purchase and bare module costs are $33,408 and $205,920 respectively.

H – 209

Heat Exchanger 209 is a single-pass shell and tube heat exchanger condenser that condenses the vapor and releases the stream back into the distillation column D-203 using refrigerant. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 600 square feet, and installed weight 18,324 lbs. The purchase and bare module costs are $12,391 and $74,390, respectively.

H – 210

Heat Exchanger 210 is a single-pass shell and tube heat exchanger reboiler that boils the liquid and releases the stream back into the distillation column D-203 using steam. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 163 square feet, and installed weight 7,746 lbs. The purchase and bare module costs are $9,422 and $55,637 respectively.

H – 301

Heat Exchanger 301 is a single-pass shell and tube heat exchanger which receives stream S-307 at 337 degrees Fahrenheit and releases stream S-310 at 175 degrees Fahrenheit using cooling water. The tube and shell are made of carbon steel. This heat exchanger condenses acrylic acid after the reaction. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 795 square feet, and its installed weight 21,450 lbs. The purchase and bare module costs are $24,500 and $77,700, respectively.

H – 302

Heat Exchanger 302 is a single-pass shell and tube heat exchanger which receives stream S-314 at 346 degrees Fahrenheit and releases stream S-320 at 100 degrees Fahrenheit cooling water. The tube and shell are made of carbon steel. This heat exchanger condenses acrylic acid after it passes through the distillation column. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 470 square feet, and its installed weight 14,500 lbs. The purchase and bare module costs are $11,500 and $36,400, respectively.

H – 303

Heat Exchanger 303 is a single-pass shell and tube heat exchanger condenser that condenses the vapor and releases the stream back into the distillation column D-301 using cooling water. The tube and shell are made of carbon steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 230 square feet, and installed weight 10,890 lbs. The purchase and bare module costs are $18,600 and $59,000, respectively.

H – 304

Heat Exchanger 304 is a single-pass shell and tube heat exchanger reboiler that boils the liquid and releases the stream back into the distillation column D-301 using steam. The tube and shell are made of stainless steel. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 2400 square feet, and installed weight 40,711 lbs. The purchase and bare module costs are $26,065 and $145,460 respectively.

8.3.3 Flash Vessels

<u>F – 201</u>

Flash vessel 201 removes CO through the top for recycling back into the process and sends to the bottoms ethylene oxide and a small amount of remaining CO. The pressure of the vessel is 614.7 psi, and the output temperature is 24.8 F. The purchase and bare module costs are 72,615.00 and 302,078.40 USD, respectively.

<u>F – 202</u>

Flash vessel 202 removes evaporated CO and EO through the top for purging and sends to the bottoms ethylene oxide and a small amount of remaining CO to be recycled back into the reactors. The splitting streams S-233, S-234, and S-235 correspond each to S-202, S-205, and S-208 respectively. The pressure of the vessel is 614.7 psi, and the output temperature is 176 F. The purchase and bare module costs are 72,615.00 and 302,078.40 USD, respectively.

<u>F – 301</u>

Flash vessel 301 allows for the second addition of MEHQ inhibitor to the process. A Nitrogen purge stream is used to capture any excess free radicals in the product acrylic acid stream. This serves to further inhibit any polymerization reactions. The estimated purchase and bare module costs are 15,880 and 48,430 USD, respectively.

8.3.4 Distillation Columns

<u>D – 101</u>

Distillation column 101 is a 12 stage column made out of Stainless Steel 304 steel designed for the ethylene oxide absorption. Tray efficiencies are specified at 70 percent for valve trays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The feed streams are S-108 and S-109. The column has no reflux, and a column diameter of 6 feet. The purchase and bare module costs are 205,335 and 854,194 USD, respectively.

<u>D – 102</u>

Distillation column 102 is a 4 stage column made out of Stainless Steel 304 designed for the purpose of stripping EO. Tray efficiencies are specified at 70 percent for valve trays with a

0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-110, enters the column at stage 1. The column no reflux ratio, and a column diameter of 6 feet. The purchase and bare module costs are 121,905 and 507,127 USD, respectively.

<u>D – 103</u>

Distillation column 103 is a 42 stage column made out of Stainless Steel 304. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-114, enters the column at stage 10. The column has a mass reflux ratio of 3.94 and a column diameter of 12 feet. The purchase and bare module costs are 959,172 and 3,990,157 USD, respectively.

<u>D – 104</u>

Distillation column 104 is a 15 stage column made out of Stainless Steel 304. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-115, enters the column at stage 11. The column has a mass reflux ratio of 1.44 and a column diameter of 5 feet. The purchase and bare module costs are 149,800 and 623,185 USD, respectively.

<u>D – 201</u>

Distillation column 201 is a 22 stage column made out of Stainless Steel 316 steel designed for the purpose of separate ethylene oxide, CO, and acetaldehyde to the distillate and β-propiolactone and sulfolane to the bottoms. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 18 inches of spacing. The liquid feed stream, S-213, enters the column at stage 15. The column has a mass reflux ratio of 0.220529. From stage 1 to 14, it has a column diameter of 3.452 feet. From stage 15 to 22, it has a column diameter of 21.371 feet. The purchase and bare module costs are $1,040,926 and $4,330,202, respectively.

<u>D – 202</u>

Distillation column 202 is an 11 stage column made out of Stainless Steel 316 designed for the purpose of separate ethylene oxide, CO, and acetaldehyde to the distillate and β-propiolactone and sulfolane to the bottoms. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-213, enters the column at stage 5. The column has a mass reflux ratio of 1.8 and a column diameter of 9.820 feet. The purchase and bare module costs are 288,649.27 and 1,200,780.97 USD, respectively.

<u>D – 203</u>

Distillation column 203 is a 16 stage column made out of Stainless Steel 316 designed for the purpose of separate ethylene oxide, CO, and acetaldehyde to the distillate and β-propiolactone and sulfolane to the bottoms. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-228, enters the column at stage 9. The column has a mass reflux ratio of 1.1 and a column diameter of 3.126 feet. The purchase and bare module costs are 102,719.59 and 427,313.50 USD, respectively.

<u>D – 301</u>

Distillation column 301 is a 16 stage column made out of carbon steel designed for the purpose of removing un-reacted β-propiolactone from the acrylic acid product stream. Tray efficiencies are specified at 70 percent for Koch flexitrays with a 0.15 psi pressure drop per stage and 24 inches of spacing. The liquid feed stream, S-313, enters the column at stage 7. The column has a mass reflux ratio of 1.2 and a column diameter of 5.5 feet. Design specifications were used to attain a mass purity and a mass recovery of 0.99 and 0.995, respectively. The estimated purchase and bare module costs are 113,660 and 427,840 USD, respectively.

8.3.5 Reactors

<u>R-101</u>

Reactor 101 is a microchannel reactor made out of stainless steel 304. It operates at 482ºF and 290 psia. The main reaction is the epoxidation of ethylene to ethylene oxide. The main side product is CO_2 with trace amounts of acetaldehyde and formaldehyde. Argon and methane are naturally in the system as impurities from the ethylene and oxygen feed. The residence time in the catalyst area is .5 seconds. The single pass conversion is 20% and the overall conversion is

82%. The raw material stream S-104 enters the reactor in a gaseous phase. The exit stream is quenched immediately with steam to get the ethylene and EO out of the flammability region. The approximate cost of the reactor is $135M. A detailed design is given in the appendix.

R – 201

Reactor 201 is a CSTR made out of Stainless Steel 316, and operates at a pressure of 614.7 psi and 176 F. Its main reaction is the production of β-propiolactone from CO and ethylene oxide, with acetaldehyde as side products. The reactor has a residence time of 0.198 hours, and is able to reach a single-pass conversion of about 90 percent. The ethylene oxide stream S-201 enters the reactor as a liquid. Recycled ethylene oxide enters through S-202. The recycled solvent sulfolane with catalyst enters the through S-203. CO input is pneumatically pressure-controlled, and is sparged into the reactor. A small gas purge stream with a flow rate of 1 lbmol/hr is on the top in order to prevent the accumulation of impurities. The products exit through the stream S-210. The heat exchanger for the reactor wraps around the reactor, and parts of it enters the reactor as well in order to ensure maximum heat exchange. The purchase and bare module costs are $92,600 and $282,425, respectively. The cost of the agitator used to stir the reactor is $3,768.79. The purchase and bare module costs of the heat exchanger are $23,092.56 and $152,583.96, respectively. The total bare module cost is $438,777.75.

R – 202

Reactor 202 is a CSTR made out of Stainless Steel 316, and operates at a pressure of 614.7 psi and 176 F. Its main reaction is the production of β-propiolactone from CO and ethylene oxide, with acetaldehyde as side products. The reactor has a residence time of 0.198 hours, and is able to reach a single-pass conversion of about 90 percent. The ethylene oxide stream S-204 enters the reactor as a liquid. Recycled ethylene oxide enters through S-205. The recycled solvent sulfolane with catalyst enters the through S-206. CO input is pneumatically pressure-controlled, and is sparged into the reactor. A small gas purge stream with a flow rate of 1 lbmol/hr is on the top in order to prevent the accumulation of impurities. The products exit through the stream S-211. The heat exchanger for the reactor wraps around the reactor, and parts of it enters the reactor as well in order to ensure maximum heat exchange. The purchase and bare module costs are $92,600 and $282,425, respectively. The cost of the agitator used to stir the reactor is \$3,768.79. The purchase and bare module costs of the heat exchanger are \$23,092.56 and \$152,583.96, respectively. The total bare module cost is \$438,777.75.

R – 203

Reactor 203 is a CSTR made out of Stainless Steel 316, and operates at a pressure of 614.7 psi and 176 F. Its main reaction is the production of β-propiolactone from CO and ethylene oxide, with acetaldehyde as side products. The reactor has a residence time of 0.198 hours, and is able to reach a single-pass conversion of about 90 percent. The ethylene oxide stream S-207 enters the reactor as a liquid. Recycled ethylene oxide enters through S-208. The recycled solvent sulfolane with catalyst enters the through S-209. CO input is pneumatically pressure-controlled, and is sparged into the reactor. A small gas purge stream with a flow rate of 1 lbmol/hr is on the top in order to prevent the accumulation of impurities. The products exit through the stream S-212. The heat exchanger for the reactor wraps around the reactor, and parts of it enters the reactor as well in order to ensure maximum heat exchange. The purchase and bare module costs are \$92,600 and \$282,425, respectively. The cost of the agitator used to stir the reactor is \$3,768.79. The purchase and bare module costs of the heat exchanger are \$23,092.56 and \$152,583.96, respectively. The total bare module cost is \$438,777.75.

R – 301

Reactor 301 is responsible for the acid catalyzed rearrangement of β-propiolactone to acrylic acid. The vessel is charged with the requisite amount of catalyst before plant startup, so no phosphoric acid passes the reactor walls. The reactor input is liquid while the output is vapor. The vessel is made out of Hasetelloy C to protect against the corrosive nature of phosphoric acid. The reaction is run at 338 Fahrenheit at 1.93 psia. The high temperature is to assure that the boiling point of acrylic acid is at least 90 degrees Fahrenheit higher than the un-reacted β-propiolactone. The space time yield of the catalyst was 0.97 g Phosphoric Acid/g β-Propiolactone/hr. This yields a volume of 11,710 gallons with a residence time of 2.8 hours. The estimated purchase and bare module costs are \$92,600 and \$282,425, respectively. The heat duty required is 2.8 hours. The heat exchanger for this reactor wraps around the reactor, and its purchase and bare module costs are \$18,383.25 and \$108,830.09, respectively. The total purchase and bare module costs are \$110,983 and \$391,255, respectively.

8.3.6 Reflux Accumulators

C – 101

Condenser Accumulator 101 is part of the condensation system of D-103. It is made out of Stainless Steel 304 and has a volume of 3021 gal, diameter of 5.5 ft, tangent height of 17 ft, and installed weight of 22,031 lbs. The purchase and bare module costs are $58,175 and $177,432, respectively.

C – 102

Condenser Accumulator 102 is part of the condensation system of D-104. It is made out of Stainless Steel 304 and has a volume of 500 gal, diameter of 3 ft, tangent height of 8.5 ft, and installed weight of 7582 lbs. The purchase and bare module costs are $27,405 and $83,600, respectively.

C – 201

Condenser Accumulator 201 is part of the condensation system of D-201. It is made out of stainless steel 316 and has a volume of 476 gal, diameter of 3 ft, tangent height of 8.5 ft, and installed weight of 1662 lbs. The purchase and bare module costs are $33,832 and $103,189, respectively.

C – 202

Condenser Accumulator 202 is part of the condensation system of D-202. It is made out of stainless steel 316 and has a volume of 1081.1 gal, diameter of 4 ft, tangent height of 11.5 ft, and installed weight of 2851 lbs. The purchase and bare module costs are $42,225 and $128,785, respectively.

C – 203

Condenser Accumulator 203 is part of the condensation system of D-203. It is made out of stainless steel 316 and has a volume of 476 gal, diameter of 3 ft, tangent height of 8.5 ft, and installed weight of 1662 lbs. The purchase and bare module costs are $33,832 and $103,189, respectively.

C – 301

Condenser Accumulator 301 is part of the condensation system of D-301. It is made out of carbon steel and has a volume of 720 gal. The purchase and bare module costs are $19,290 and $58,830, respectively.

8.3.7 Storage Tanks

ST – 301

Storage tank 301 was sized based on the assumption that product would be shipped every other day. The acrylic acid is stored under a pressure of 50 psia and a temperature of 77ºF with small amounts of oxygen to facilitate the MEHQ inhibitor mechanism. The material is stainless steel with estimated purchase and bare module costs of 557,550 and 1,700,527 USD, respectively.

8.3.8 Vacuum Systems

V-201

Vacuum 201 is used to maintain the pressure of distillation column D-201 at 3.7 psia. The leak rate is 227.523 lb/hr. The bare module cost is 8,321.35 USD.

V-202

Vacuum 201 is used to maintain the pressure of distillation column D-203 at 2 psia. The leak rate is 207.940 lb/hr. The bare module cost is 18,930.67 USD.

V-301

Vacuum system 301 is responsible for maintaining reactor 301 at a pressure of 1.93 psia for the β-propiolactone rearrangement. The air leakage rate was calculated to be 16.2 lb/hr with a vapor flow of 20 lb/hr. Adding these two values together gives a total flow to the vacuum of 36.2 lb/hr.

8.3.9 Compressors

K-201

Compressor 201 is used to increase pressure of stream S-214 before it enters distillation D-203. It increases the pressure from 3.7 psia to 17 psia, and uses 256.945 Hp or motor power. The purchase and bare module costs are 165,851.57 and 605,504.22 USD, respectively.

Section 9 - Conclusions

Based on the cost-plus economic analysis completed, with an IRR of 42.17% and an NPV of $288M, the ethylene based acrylic acid is feasible and a potential threat to the propylene based business. The 2-step process analysis showed the potential of decreasing ethylene and EO prices to increase the profitability of the second two steps enormously.

To investigate the ethylene based process and evaluate it properly, further technical analysis is needed. Further design work must be done to properly size and cost the microchannel reactor. Since the microchannel reactor alone costs 50% of all the equipment, it is the unit that could make or break the EO process. The microchannel reactor needs to be run in a pilot plant setting vs a lab setting to better analyze the true efficiency of the microchannels. It is important to note that for this report, the microchannels were run at 90% selectivity as seen in industry at 20% per pass conversion. However, patent 0036106 A1 describes an embodiment in which they achieve 50% per pass conversion at 80% selectivity. With the use on an industrial catalyst at a constant operating temperature range, it may be possible to achieve a selectivity as high as 90%, and with a 50% per pass conversion, downstream equipment would be considerable smaller and utilities would be considerably cheaper, making the ethylene based acrylic acid even more plausible. Further design will have to be conducted on the carbonylation CSTR in a pilot plant to properly extract kinetic data and apply them to this process. Also, a pilot plant study on the necessary ratio of β-lactone to phosphoric acid ratio. These factors could potentially decrease residence times, reactor volumes, downstream column sizing, and utilities.

This preliminary project has an IRR of 13.86% with a NVP of -$50M after a capital cost of over $550M. The viability of the microchannel reactor is directly tied to the large variability in its costs. At this time, the microchannel system cannot offer benefits and outweigh its costs. What is also clear after is that this project depends directly on the cost of ethylene and ethylene oxide. With the expectation of ethylene costs dropping, this project confirms the threat posed to the propylene based industry. The group highly recommends further studies and investigation of the technologies involved in this process.

Section 10 – Acknowledgements

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- Mr. John Wismer for suggesting the project and providing us with patents and sources for kinetic data as well as costing and sizing information
- The industrial consultants for helping us brainstorm ideas and develop our processes

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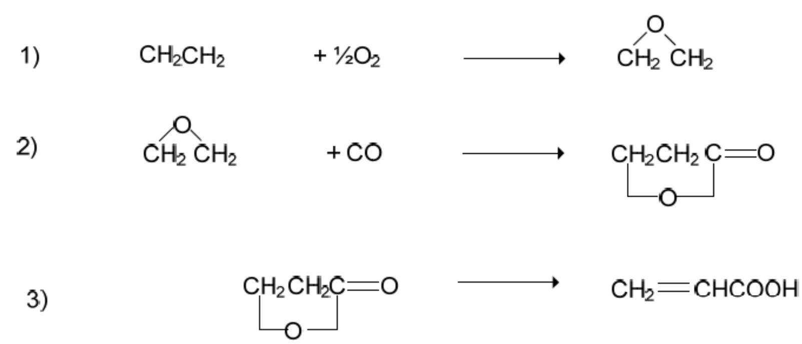
Appendix

APPENDIX A: Problem Statement

2. Acrylic Acid from Ethylene
(recommended by John A. Wismer, Arkema)

The global market for acrylic acid (AA) exceeds 10 billion pounds/year. In developed countries, demand is growing faster than GDP thanks to a healthy growth in acrylic resins and superabsorbent polymers. Most of the world's production capacity uses propylene as a precursor with acrolein being the key intermediate. However, AA can also be made from ethylene. Historically, propylene has sold at a slight discount to ethylene due to its ready availability as a by-product of refinery cracking operations. In recent years, the market dynamics in the US have started to shift in response to two trends that are projected to continue in the coming years. The first is near-zero growth in US refinery production in the face of competition from foreign "megarefineries" and a hostile regulatory environment. This is taking place in spite of an increase in domestic oil production. The second trend is the increasing availability of ethane from shale gas as a feedstock to ethylene crackers. As the new ethane crackers force the shutdown of the higher cost naphtha units, lower ethylene prices should follow.

Your client is interested in knowing whether ethylene derived acrylic acid will be a threat to its propylene based manufacturing platform. The proposed route to acrylic acid from ethylene proceeds in three steps.



The first step is a direct oxidation of ethylene to ethylene oxide. Purveyors of relatively new microchannel reactor technologies have made EO a target process[1,2,3]. Microchannel reactor technology enables the process to operate safely in the flammable region and controls reactor temperatures within a narrow range to improve selectivity. Evaluate this technology and use on the first step if appropriate. Design details for microchannel reactors can be found in previous senior design project reports[10].

The second step is a carbonylation of ethylene oxide to beta-propriolactone. This is typically a liquid phase catalyzed reaction. The carbon monoxide reactant is available by pipeline on the Gulf Coast. This reaction can proceed in a number of solvents, but there are obvious advantages to high-boiling solvents such as sulfolane. The catalyst is presumably homogeneous. It typically is comprised of carbonyl cobaltate and a metal centered Lewis acid. All patent examples are based on batch reactors[6]. Part of the design challenge is to extract kinetic data from the batch results so that CSTR-based configurations can be evaluated. The major non-selective is succinic anhydride- a result of the carbonylation of the lactone. There are indications that succinic anhydride can be greatly reduced or eliminated by reactor design and/or manipulation of process conditions.[7,8]

The final step is an acid catalyzed rearrangement of beta-lactone to acrylic acid. This reaction is highly selective as long as an inhibitor is used to prevent polymerization of the acrylic acid[9]. There are suggestions of process intensification by close coupling the carbonylation and rearrangement reactions to avoid propriolactone isolation. The toxicity of propriolactone and its susceptibly to decomposition at its normal boiling-point provide strong incentives for avoiding its isolation.

The acrylic acid project should produce 300 million pounds/year. Ethylene pricing should be "cost plus" based on quoted prices for ethane. This should give significantly lower prices than the current market price of ethylene, which will hold up as long as naphtha based crackers supply a significant portion of domestic ethylene.

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APPENDIX B: Calculations

Costing

Sample Shell and Tube Price Calculation: H-301

Shell and Tube Floating Head Heat Exchanger with 800 ft^2 area. Shell and Tube materials are Carbon Steel with 20 ft tube length.

$f.o.b\ Purchase\ Cost\ C_P = F_P F_M F_L C_B$

$Floating\ Head\ C_B = \exp(11.667 - 0.8709[\ln(A)] + 0.09005[\ln(A)^2])$

$C_B = \exp(11.667 - 0.8709[\ln(800)] + 0.09005[\ln(800)^2])$

$C_B = 19,325.3$

$F_P = 0.9803 + 0.018[\frac{P}{100}] + 0.0017[\frac{P}{100}]^2$

$F_P = 0.9803 + 0.018[\frac{80}{100}] + 0.0017[\frac{80}{100}]^2$

$F_P = 1.00$

$F_L = 1.00$

$F_M = a + [\frac{A}{100}]^b$

For Carbon Steel/Carbon Steel $a = 0.00, b = 0.00$

$F_M = 1.00$

$C_P = \$24,500$

Sample Distillation Tower Price Calculation: D-301

Valve trays are used so $F_{TT} = 1.18$. The material is carbon steel so $F_{TM} = 1.0$. The tower has 14 trays with a diameter of 5.5 ft.

$C_P = F_M C_V + C_{PL} = 1.0(68,592) + 17,813 = \$86,405$

$W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho$

$W = \pi(5.5 + 0.0144)(42 + 0.8(5.5))(0.0144)(490) = 14,552lb$

$C_V = \exp(7.2756 + 0.18255[\ln(W)]) + 0.02297[\ln(W)]^2)$

$C_V = \exp(7.2756 + 0.18255[\ln(14552)]) + 0.02297[\ln(14552)]^2) = \$68,592$

$C_{PL} = 300.9(D_i)^{0.63316}(L)^{0.80161}$

$C_{PL} = 300.9(5.5)^{0.63316}(42)^{0.80161} = \$17,813$

Calculate Tray Costs and add this to the purchase cost.

$C_{BT} = 468\exp(0.1739D_i) = 468\exp(0.1739(5.5)) = 1217.93$

$F_{NT} = \frac{2.25}{1.0414^{NT}} = \frac{2.25}{1.0414^{14}} = 1.275$

$C_T = N_T F_{NT} F_{TT} C_{BT} = (14)(1.275)(1.18)(1217.93) = \$27,257$

Purchase Cost $= C_P + C_T = \$113,662$

Total Bare Module Cost $= F_{BM}(C_P + C_T) = (4.16)(113,662) = \$472,837$

Centrifugal Pumps: P-301

Pump 301 is made of Cast Iron with a flow rate of 78.5 gpm and a fluid head of 90.95 ft.The Type Factor $F_T = 1.0$ and the material factor $F_M = 1.0$

$S = Q(H)^{0.5} = (78.5)(90.95)^{0.5} = 748.64$

$C_B = exp(9.7171 - 0.6019[\ln(S)] + 0.0519[ln(S)]^2)$

$C_B = exp(9.7171 - 0.6019[\ln(748.64)] + 0.0519[ln(748.64)]^2) = \$3001.5$

$C_P = F_T F_M C_B$

$C_P = (1.0)(1.0)(3001.5) = \$3001.5$

Calculate Bare Module Cost

$C_{BM} = C_P F_{BM} = (3001.5)(3.3) = \$9,904.44$

Vacuum System: VC-301

Vacuum 301 is responsible for mainting the reactor vessel 301 at 100 torr. The reactor has a volume of 1566 ft^3.

Calculate the Air Leakage Rate W

$W = 5 + (0.0298 + 0.03088[\ln(P)] - 0.0005733[\ln(P)]^2)V^{0.66}$

$W = 5 + (0.0298 + 0.03088[\ln(100)] - 0.0005733[\ln(100)]^2)(1566)^{0.66} = 40\frac{lb}{hr}$

Sizing

Sample Storage Tank Sizing: ST-301

ST-301 holds the final acrylic acid product. Allow 10% headspace for oxygen. The product flow rate is $37{,}360\frac{lb}{hr}$. The holding time is assumed to be 2 days or 48 hours.

$Volume = \frac{(Flowrate)(HoldingTime)}{0.8(\rho_{Acid})}$

$Volume = \frac{(37{,}360)(48)}{0.9(64.4)} = 30,900ft^3$

$Volume = 30,900ft^3(7.48)\frac{gal}{ft^3} = 231,900gal$

Sample Pump Sizing: P-103

Reflux pump for Distillation Column D-103.Assume a 2 psi drop per 100 ft of pipe.Assume 2 control valves per side of pump with a 10 psi drop each.

$Head = (\frac{V_d^2}{2g} + Z_d + \frac{P_d}{\rho_d g}) - (\frac{V_s^2}{2g} + Z_s + \frac{P_s}{\rho_s g})$

$V_d = V_s, Z_d = Z_s, \rho_d = \rho_s$

$\Delta Z = 0$

$PipeLength = 100 + 100 + 20 = 220ft \ PressureDrop = 10(4) = 40psi$

$\Delta P = 82.2$

$\rho = 0.434[h][specificgravity]$

$Head = \frac{82.2}{0.434}\%(0.99) = 189.6ft$

Theoretical $HP = \frac{(gpm)(psi)}{1714} = \frac{(473.7)(82.2)}{1714} = 22.7HP$

Sample Tower Sizing: D-301

D-301 removes acrylic acid vapors from unreacted β propiolactone.Use $f = 0.85$ Assume 24 inch tray spacing. Use valve Trays so $F_{HA} = 1.0$. Assume a non-foaming system so $F_F = 1.0$. $\rho_G = 0.32\frac{lb}{ft^3}, \rho_L = 57.8\frac{lb}{ft^3}, \sigma = 20\frac{dyne}{cm}.L = 1453.12\frac{lb}{hr}, G = 37,327\frac{lb}{hr}$

$U_f = C[\frac{\rho_G - \rho_G}{\rho_G}]^{\frac{1}{2}} = 0.39(\frac{57.8-0.32}{0.32})^{0.5} = 4.29\frac{ft}{s}$

$C = C_{SB}F_{ST}F_F F_{HA} = (0.39)(1)(1)(1) = 0.39$

Use Figure 19.4 from Seider's Book to obtain C_{SB}.

$F_{LG} = (\frac{L}{G}\frac{\rho_G}{\rho_L})^{0.5} = \frac{1453.12}{37{,}327}[\frac{0.32}{57.8}]^{0.5} = 0.0029 \rightarrow C_{SB} = 0.39$

$F_{ST} = [\frac{\sigma}{20}]^{0.20} = [\frac{20}{20}]^{0.2} = 1$

$\frac{A_d}{A_t} = 0.1$

$D_T = [\frac{4G}{(fU_f\pi(1-\frac{A_d}{A_T})\rho_G}]^{0.5} = \frac{4(37{,}327)}{3600(0.85)(4.29)\pi(1-0.1)(0.32)} = 3.54ft$

Sample Reactor Sizing: R-301

R-301 is assumed to be a uniformly stirred tank reactor. Sizing is based on the amount of phosphoric acid in the tank.Assume as per Professor Fabiono's suggestion that the space time yield of catalyst is $0.97\frac{gramsPropiolactone}{g*H_3PO_4*hr}$

H_3PO_4 Volume $= (37,313\frac{lbLactone}{hr})(fraclbAcid * hr0.97lbLactone) = 38467$ lb Lactone

APPENDIX C: Specialty Equipment Design and Costing

This microchannel reactor is based on *Kestenbaum et al*. Several different configurations are discussed in the paper; however, a detail design of an industrial sized reactor is not discussed. Sizing details and results are only given for lab scale channels with up to 21 streams. Thus, the reactor had to be extrapolated to determine the number of channels used for their process. The process of reactor sizing is based off of the method used in *Alaskan Natural Gas to Liquids*, specifically, the Fischer-Tropsch Reactor FTR-201

Reactor Design

At a range of pressures from 2-20 bar, the typical residence time was .1-1.5 seconds, with the residence time increasing as pressure increased. ½ seconds led to the best selectivity, an assumption is that the reactor can run at 20 bar with a residence time of .5 seconds. The contact time is not defined in the paper as the contact time at STP, so it was assumed that the contact time was in terms of the temperature and pressure of the inlet stream, which was always between 250-290^{o}C and 2-20 bar.

The inlet stream enters with a flow rate of 165,106 ft^3/hr. With a contact time of .5 s (1.3889x10^{-4} hr), the reaction zone volume is 22.94 ft^3, or 6.496x10^8 mm^3.
The next necessary step was to determine the reaction zone volume per channel. The paper states that each etched catalyst area contains channels of 200um in width, 80um in height, and 9.5mm in length. Each foil contains 9 channels, and 21 foils can be stacked on top of each other to product a stack. Each stack contains 2.8728x10^{-8} m^3, or 28.728 mm^3. Therefore, 2.2612x10^7 stacks are necessary.

A void fraction of 50% was assumed for the catalyst, and the resulting total amount of stacks needed to maintain volumetric flow minimums are 4.5224x10^7 stacks.

Each stack contains a mixing area that is around the same size as the catalytic area; the only difference is that the width of the channels vary to promote mixing. For this reactor, we will assume that the overall mixing area volume is the same as the catalytic area volume. Therefore, 4.5224x10^7 mixing units will be necessary, along with 4.5224x10^7 inlet oxygen paths and 4.5224x10^7 inlet ethylene-recycle mix paths.

The cooling will occur between the stacks since one inlet stream of raw material is dispersed over the 21 foils in each stack. The amount of area for heat transfer is 90.25 mm^2 per side of each stack. The steam flow must be over the catalytic area only as to not drop the temperature of the reactants before entering the catalytic area.

To calculate the amount of heat removal necessary, it was assumed that the heat of reaction would be similar to that seen in an industrial setting, around -350 kJ/mol ethylene. With 20% of the ethylene being converted at 77.14 mol/sec, the total heat of reaction is $2.7x10^4$ W. Area of cooling is 2 sides x $4.5224x10^7$ units x 90.25 mm^2, totaling $8.0407x10^9$ mm^2. Total heat flux must be $3.31x10^{-6}$ W/mm^2 or $3.31x10^{-4}$ W/cm^2.

Reactor Costing

Microchannel reactors have not been commercialized with reliable prices. Thus, many assumptions must be made about the cost of the reactor. Using MEPS International Ltd., the average price of stainless steel 304 was $2812 / tonne in March, 2014.

Each stack will be etched, therefore they will start as a solid block of stainless steel. Each stack is 9.5 mm by 9.5 mm by 4.2 mm. The total volume per stack is 380 mm^2. The total volume of catalyst area needed is 17.15 m^3. The density of stainless steel 304 is 8030 kg/m^3. The total weight of steel needed for all catalytic area stacks is 137.72 tonnes. Similarly, the total weight of steel needed for all mixing area stacks is 137.72 tonnes.

The unit containing the mixing unit and catalytic area must now be accounted for. Referring to the scale on Figure 1 in *Kestenbaum et al.*, the unit seems to be 5 cm wide by 5 cm long. The depth must be more than the thickness of a stack which is 4.2 mm. It was assumed that the thickness is 5 mm. Thus, the volume per stack is 12.5 cm^3. For all $4.5224x10^7$ units, the total volume is 565.3 m^3, resulting in 4539 tonnes.

The total amount of stainless steel needed is 4814.44 tonnes. Since the paper only tested on stacks, there is no information regarding the potential structuring of stacks to create reactor modules. To account for the metal necessary for creating and structuring each module to hold multiple stacks, as well as add space for cooling steam, we will multiply the necessary weight of steel by 2. This results in a total weight of 9628.88. At $2812/tonne, the total material cost is $27.08M.

To account for the potentially large manufacturing costs associated with etching, laser cutting, and making such small and fine channels, *Alaskan Natural Gas to Liquids* chose a bare module factor of 5. The total bare module cost of the reactor is $135.4M.

Catalyst Costing

Catalyst costs were determined by costing the most expensive factor, silver. The catalyst is assumed to have a void fraction of ½. Therefore, it is assumed that ½ of the volume in the catalyst area will be filled with catalyst. The catalyst is Ag on α-alumina. It is assumed that the weight fraction of Ag is 15% based on the range given by *Bartholomew et al*. The total volume of the catalyst area after accounting for the catalyst void fraction of .5 is 45.88 ft^3, so the catalyst area is 22.94 ft^3. Low surface area α-alumina leads to higher selectivity, and these catalysts generally have a density of 3.97 g/cm^3. This results in a weight of 2.58 tonnes of catalyst. The BET surface area of this catalyst is around .5 m^2/g, resulting in a total surface area of 1.29×10^6 m^2. Ag makes up around 15% of the surface area, so the total surface of silver is 1.93×10^5 m^2. Each silver atom has a projected surface area of .0652 nm^2, for a total of 4.92 moles of silver. This is equivalent to 530 g. The cost per troy ounce of silver is $20.01, summing to a total cost of $342. If there are 3 layers of silver on average, the total cost of silver becomes $1000. Using a bare module factor of 20 for the purchase, installation, and disposal cost of silver and α-alumina, the total cost sums to $20000.

MEA CO_2 Removal Unit Costing

The CO_2 removal unit is based off the unit that was designed in the paper *Alaskan Natural Gas to Liquids (GTL).* The MEA system was designed in aspen for a larger gas flow rate with 80% removal. The GTL MEA system was determined to cost $967,315,790 for a GTL production capacity of 10955.87 ft^3/hr of CO_2. For the EO system, the production capacity is 74.4 ft^3/hr of CO_2. Using the economy-of-scale method, six-tenths factor, and CE indexing, the installed cost of the EO MEA system was determined to be $50,805,790.75.

APPENDIX D: Economic Analysis Tables

Equipment Costing

	Equipment Number	Name	Type	F.O.B. Purchase Cost (USD)	Bare Module Factor of Guthrie (1974)	CE Index 2014	CE Index 1974	Equipment Bare Module Cost (USD)
Block 100	C-101	Purification Tower 1 Reflux Drum	Fabricated Equipment	58174.51	3.05	525	275	338734.29
	C-102	Purification Tower 2 Reflux Drum	Fabricated Equipment	27405.97	3.05	525	275	159577.47
	D-101	EO Absorber	Fabricated Equipment	205335.04	4.16	525	275	1630733.55
	D-102	EO Stripper	Fabricated Equipment	121905.66	4.16	525	275	968152.58
	D-103	Purification Tower 1	Fabricated Equipment	959172.40	4.16	525	275	7617572.78
	D-104	Purification Tower 2	Fabricated Equipment	149804.07	4.16	525	275	1189716.72
	H-101	Inlet Gas Heater	Fabricated Equipment	21412.90	3.17	525	275	129586.96
	H-102	Outlet Gas Cooler	Fabricated Equipment	35094.98	3.17	525	275	212388.44
	H-103	Purification Tower 1 Feed Stream Cooler	Fabricated Equipment	58680.26	3.17	525	275	355122.26
	H-104	Recycle Water Cooler	Fabricated Equipment	54962.55	3.17	525	275	332623.37
	H-105	Steam Quench Heater	Fabricated Equipment	16058.33	3.17	525	275	97182.08
	H-106	EO Stripper Reboiler	Fabricated Equipment	343826.28	3.17	525	275	2080774.14
	H-107	Purification Tower 1 Reboiler	Fabricated Equipment	46640.59	3.17	525	275	282260.39
	H-108	Purification Tower 2 Reboiler	Fabricated Equipment	14211.20	3.17	525	275	86003.61
	H-109	Purification Tower 1 Condenser	Fabricated Equipment	102288.36	3.17	525	275	619030.54
	H-110	Purification Tower 2 Condenser	Fabricated Equipment	15347.09	3.17	525	275	92877.79
	P-101	Recycle Water Pump	Process Machinery	5068.21	3.3	525	275	31929.72
	P-102	Purification Tower 1 Reflux Pump	Process Machinery	4640.29	3.3	525	275	29233.80
	P-103	Purification Tower 2 Reflux Pump	Process Machinery	3121.51	3.3	525	275	19665.54
	R-101	Microchannel Reactor system	Fabricated Equipment	N/A	N/A	525	275	135400000.00
	CO2SCRUB	MEA CO2 Scrubbing Unit based on GTL	Fabricated Equipment	N/A	N/A	525	275	50805790.75
		Note: MEA Installed Cost is calculated using Economy-of-Scale and Six-Tenths Factor						

	Equipment Number	Name	Type	F.O.B. Purchase Cost (USD)	Bare Module Factor of Guthrie (1974)	CE Index 2014	CE Index 1974	Equipment Bare Module Cost (USD)
Block 200	H-204	Distillation Column D – 201 Condenser	Fabricated Equipment	19826.98	3.17	525	275	119989.27
	H-205	Distillation Column D – 201 Reboiler	Fabricated Equipment	28439.54	3.17	525	275	172110.90
	H-206	Distillation Column D – 202 Condenser	Fabricated Equipment	72291.23	3.17	525	275	437493.38
	H-207	Distillation Column D – 202 Reboiler	Fabricated Equipment	56290.88	3.17	525	275	340662.16
	H-208	Distillation Column D – 203 Condenser	Fabricated Equipment	28439.55	3.17	525	275	172110.98
	H-209	Distillation Column D – 203 Reboiler	Fabricated Equipment	13503.38	3.17	525	275	81720.02
	F-201	CO Purge vessel	Fabricated Equipment	59683.06	4.16	525	275	473992.03
	F-202	EO and CO purge vessel	Fabricated Equipment	59683.06	4.16	525	275	473992.03
	H-203	Ethylene Oxide Heater	Fabricated Equipment	9364.06	3.17	525	275	56669.60
	H-202	β-Propiolactone cooler	Fabricated Equipment	69726.20	3.17	525	275	421970.30
	H-203	β-Propiolactone condenser	Fabricated Equipment	20413.72	3.17	525	275	123540.12
	K-201	Distillation Column 3 feed compressor	Process Machinery	134312.96	4.16	525	275	1066689.10
	D-201	Distillation Column 1	Fabricated Equipment	1040926.04	4.16	525	275	8266845.36
	D-202	Distillation Column 2	Fabricated Equipment	102719.59	4.16	525	275	815780.32
	D-203	Distillation Column 3	Fabricated Equipment	13503.38	3.17	525	275	81720.02
	R-201	CSTR Reactor 1	Fabricated Equipment	292008.53	4.16	525	275	2319078.67
	R-202	CSTR Reactor 2	Fabricated Equipment	292008.53	4.16	525	275	2319078.67
	R-203	CSTR Reactor 3	Fabricated Equipment	292008.53	4.16	525	275	2319078.67
	V-201	Distillation Column 1 Vacuum	Fabricated Equipment	8321.35	1	525	275	15886.22
	V-202	Distillation Column 2 Vacuum	Fabricated Equipment	18930.67	1	525	275	36140.37
	P-201	Distillation Column D-201 reflux pump	Process Machinery	5708.52	3.3	525	275	35963.67
	P-202	Distillation Column D-202 reflux pump	Process Machinery	3049.79	3.3	525	275	19213.68
	P-203	Distillation Column D-203 reflux pump	Process Machinery	2964.23	3.3	525	275	18674.68
	C-201	Condenser Accumulator D-201	Fabricated Equipment	33832.49	3.05	525	275	196997.39
	C-202	Condenser Accumulator D-202	Fabricated Equipment	42224.58	3.05	525	275	245862.21
	C-203	Condenser Accumulator D-203	Fabricated Equipment	33832.49	3.05	525	275	196997.39

	Equipment Number	Name	Type	F.O.B. Purchase Cost (USD)	Bare Module Factor of Guthrie (1974)	CE Index 2014	CE Index 1974	Equipment Bare Module Cost (USD)
Block 300	F-302	Flash purification of Acrylic Acid Product	Fabricated Equipment	15879.95	3.05	525	275	92464.64
	H-301	Reactor outlet condenser	Fabricated Equipment	24523.05	3.17	525	275	148409.06
	H-302	Acrylic Acid Condenser	Fabricated Equipment	11489.47	3.17	525	275	69532.18
	P-301	Feed pump for D-301	Process Machinery	3001.35	3.3	525	275	18908.48
	P-302	Storage Pump	Process Machinery	2983.09	3.3	525	275	18793.48
	C-301	Reflux Accumulator for D-301	Fabricated Equipment	22195.79	4.16	525	275	176274.89
	H-303	Condenser for D-301	Fabricated Equipment	18591.56	3.17	525	275	112512.75
	K-301	Reboiler for D-301	Fabricated Equipment	26065.35	3.17	525	275	157742.78
	R-301	Beta-Propiolactone to Acrylic Acid Reactor	Fabricated Equipment	107924.10	3.05	525	275	628412.60
	D-301	Distillation Tower for Acrylic Acid	Fabricated Equipment	112447.73	4.16	525	275	893039.45
	P-303	Reflux Pump for D-301	Process Machinery	2965.27	3.3	525	275	18681.22
	V-301	Reactor Vacuum	Fabricated Equipment	30003.71	1	525	275	57279.81
	F-303	Flash to Vacuum System	Fabricated Equipment	17306.40	3.05	525	275	100770.46
	ST-301	Acrylic Acid storage tank	Fabricated Equipment	144394.04	1	525	275	275661.35

	Total Cost Fabricated Equipment and Process Machinery	**226,075,697.10**

Economics Spreadsheets Total Process

Total Capital Investment

Total Cost Fabricated Equipment and Process Machinery	**$226,075,697.10**
Cost of Spares	$45,215,139.42
Initial Catalyst Charge	$996,000.00
Cost for Computers and software	$10,000,000.00
Total Bare Module Investment	**$282,286,836.52**
Site Preparation	$13,564,541.83
Service Facilities	$11,303,784.85
Allocated costs for Utilities:	
Steam	$17,425,359.24
Electricity	$2,901,362.08
Cooling Water	$983,933.72
Process Water	$29,829.74
Refrigeration	$5,840,528.22
Total Allocated Costs for Utilities and Related Facilities	**$27,181,013.01**
Direct Permanent Investment	**$334,336,176.21**
Cost of Contingencies and Contractors Fees	**$117,017,661.67**
Total Depreciable Capital	**$451,353,837.88**
Land	$9,027,076.76
Initial Royalty Fee	$9,027,076.76
Cost for Start-up	$45,135,383.79
Site Factor - Gulf Coast	1
Total Permanent Investment	**$514,543,375.19**
Working Capital:	
Cash Reserves - 1 Month	$6,524,789.08
Inventories for Products - 1 Week	$5,769,230.77
Accounts Receivable	$25,000,000.00
Accounts Payable	$7,399,371.31
Total Working Capital	$44,693,391.16
Total Capital Investment	**$559,236,766.35**

Utilities

	Name	Fluid	Rate	Rate Units	Cost	Units	Cost per Hour	Cost Units	Total Yearly Cost
STEP 1	Electricity		162.355	KW	$ 0.06	USD/KW-H	$9.74	USD/H	$81,826.92
	Cooling Water	Water	507175	GAL/H	$ 0.08	USD/1000gal	$38.04	USD/H	$319,520.25
	Process Water Start Up	Water	22525	GAL	$ 0.75	USD/1000gal	$16.89	USD	$16.89
	Process Water	Water	22.525	GAL/H	$ 0.75	USD/1000gal	$0.02	USD/H	$141.91
	Refrigerant - Propane	Refrigerant	261.3359	KLB/H	$ 0.07	USD/Ton-H	$9.26	USD/H	$77,747.43
	Refrigerant - Freon 12	Refrigerant	1064.454	KLB/H	$ 0.10	USD/Ton-H	$53.22	USD/H	$447,070.68
	Steam @100PSI	Steam	108.3391	KLB/H	$ 4.14	USD/1000lbs	$448.52	USD/H	$3,767,600.54
	Steam @165PSI	Steam	86.3409	KLB/H	$ 4.96	USD/1000lbs	$428.25	USD/H	$3,597,307.26
	Steam @400PSI	Steam	20.97	KLB/H	$ 6.41	USD/1000lbs	$134.35	USD/H	$1,128,547.74
	Dirty Water Removal								
STEP 2	Electricity		898.235	KW	$ 0.06	USD/KW-H	$53.89	USD/H	$452,710.44
	Cooling Water	Water	712617	GAL/H	$ 0.08	USD/1000gal	$53.45	USD/H	$448,948.71
	Refrigerant - Propane	Refrigerant	4.74008	KLB/H	$ 0.07	USD/Ton-H	$0.17	USD/H	$1,410.17
	Refrigerant - Freon 12	Refrigerant	48.5794	KLB/H	$ 0.10	USD/Ton-H	$2.43	USD/H	$20,403.35
	Steam @100PSI	Steam	4.60524	KLB/H	$ 4.14	USD/1000lbs	$19.07	USD/H	$160,151.83
STEP 3	Electricity		80.668	KW	$ 0.06	USD/KW-H	$4.84	USD/H	$40,656.67
	Cooling Water	Water	292277	GAL/H	$ 0.08	USD/1000gal	$21.92	USD/H	$184,134.51
	Steam @400PSI	Steam	20.71821	KLB/H	$ 6.41	USD/1000lbs	$132.80	USD/H	$1,115,551.30
						Total Utility Costs (CE adjusted)			**$12,435,933.93**

Total Fixed Costs

Utilities	**Total Utility Costs**	**$12,435,933.93**
Labor-related Operations	Days of Operation	350
	Hours of operation per year	8400
	Hours of operation per week	168
	Operator hours per week	40
	Operators shifts per week	4.2
	Assumed Operators shifts per week	5
	Number of sections	3
	Operators per section table 23.3	1
	Operator Manager	1
	Total operators per shift	4
	Hours per shift	8
	Weeks of operation	50
	Wage	$35.00
	Texas/Gulf cost factor	1
	Direct wages & benefits	$1,400,000.00
	Direct salaries & benefits	$210,000.00
	Operating supplies and services	$84,000.00
	Technical assistance to manufacturing	$300,000.00
	Control laboratory	$325,000.00
	Total Operations Annual Cost, O	**$2,319,000.00**
Maintenance	Total Depreciable Capital - from TCI page	$451,353,837.88
	Maintenance wage & benefits	$18,956,861.19
	Salaries & benefits	$5,687,058.36
	Materials & services	$22,748,233.43
	Maintenance overhead	$1,137,411.67
	Total Annual Maintenance Costs, M	**$48,529,564.65**
Operating Overhead	DW&B	$1,400,000.00
	Direct salaries and benefits	$210,000.00
	MW&B	$18,956,861.19
	Maintenance salaries and benefits	$5,687,058.36
	Total Annual M&O-SW&B	**$26,253,919.55**
	General plant overhead	$1,864,028.29

	Mechanical department services	$630,094.07
	Employee relations department	$1,548,981.25
	Business services	$1,942,790.05
	Total Annual Operating Overhead, O	**$5,985,893.66**
Property Taxes & Insurance	**Total Property Taxes & Insurance**	**$9,027,076.76**
Depreciation	Please see MACRS depreciation in Cash Flow (not included in COM)	
	Total Cost of Manufacture, COM	**$78,297,468.99**
	Total Fixed Costs	**$78,297,468.99**

Total Variable Costs and Total Revenues

	Name	**Cost**	**Unit**	**lbs/yr**	**Total Cost**
Raw Materials	Ethylene	$0.46	USD/lb	150494400	$69,227,424.00
	Oxygen	$0.05	USD/lb	123916800	$6,195,840.00
	CO2 Removal solvents/MEA	$0.31	USD/barrel EO	679603.428	$210,677.06
	Carbon Monoxide	$0.10	USD/lb	126545146.6	$12,654,514.66
	MEHQ	$5.00	USD/lb	100800	$504,000.00
				Cost of Raw Materials	**$88,792,455.72**
Product Sales	Acrylic Acid	$1.00	USD/lb	300000000	$300,000,000.00
General Expenses					
	Selling/Transfer expense		3%		
	Direct Research		4.8%		
	Allocated Research		0.5%		
	Administrative Expenses		2%		
	Management incentive compensation		1.25%		
	Total General Expenses as a function of Revenues		12%		$36,000,000.00
Total Variable Costs					**$124,792,455.72**
Total Variable Revenues					**$300,000,000.00**

Cash Flow

Year	Plant Capacity	Total Capital Investment	Catalyst Charge	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2015	0%	-$559,236,766.35							-$559,236,766.35	$0.00	$0.00	-$559,236,766.35
2016	50%			0.2	-$90,270,767.58	-$78,297,468.99	-$62,396,227.86	$150,000,000.00	$9,306,303.15	$0.00	$0.00	$9,306,303.15
2017	100%			0.32	-$144,433,228.12	-$80,646,393.06	-$128,536,229.39	$309,000,000.00	$99,817,377.55	$0.00	$0.00	$99,817,377.55
2018	100%			0.192	-$86,659,936.87	-$83,065,784.85	-$132,392,316.27	$318,270,000.00	$102,811,898.87	$16,151,962.00	-$6,460,784.80	$96,351,114.07
2019	100%			0.1152	-$51,995,962.12	-$85,557,758.40	-$136,364,085.76	$327,818,100.00	$105,896,255.84	$53,900,293.72	-$21,560,117.49	$84,336,138.35
2020	100%			0.1152	-$51,995,962.12	-$88,124,491.15	-$140,455,008.33	$337,652,643.00	$109,073,143.51	$57,077,181.39	-$22,830,872.56	$86,242,270.96
2021	100%		-$966,000.00	0.0576	-$25,997,981.06	-$90,768,225.89	-$144,668,658.58	$347,782,222.29	$111,379,337.82	$85,381,356.76	-$34,152,542.70	$77,226,795.12
2022	100%					-$93,491,272.66	-$149,008,718.34	$358,215,688.96	$115,715,697.95	$115,715,697.95	-$46,286,279.18	$69,429,418.77
2023	100%					-$96,296,010.84	-$153,478,979.89	$368,962,159.63	$119,187,168.89	$119,187,168.89	-$47,674,867.56	$71,512,301.34
2024	100%					-$99,184,891.17	-$158,083,349.29	$380,031,024.42	$122,762,783.96	$122,762,783.96	-$49,105,113.58	$73,657,670.38
2025	100%					-$102,160,437.90	-$162,825,849.77	$391,431,955.15	$126,445,667.48	$126,445,667.48	-$50,578,266.99	$75,867,400.49
2026	100%		-$966,000.00			-$105,225,251.04	-$167,710,625.26	$403,174,913.80	$129,273,037.50	$129,273,037.50	-$51,709,215.00	$77,563,822.50
2027	100%					-$108,382,008.57	-$172,741,944.02	$415,270,161.22	$134,146,208.63	$134,146,208.63	-$53,658,483.45	$80,487,725.18
2028	100%					-$111,633,468.83	-$177,924,202.34	$427,728,266.05	$138,170,594.89	$138,170,594.89	-$55,268,237.95	$82,902,356.93
2029	100%					-$114,982,472.89	-$183,261,928.41	$440,560,114.04	$142,315,712.73	$142,315,712.73	-$56,926,285.09	$85,389,427.64
2030	100%					-$118,431,947.08	-$188,759,786.26	$453,776,917.46	$146,585,184.12	$146,585,184.12	-$58,634,073.65	$87,951,110.47
2031	100%		-$966,000.00			-$121,984,905.49	-$194,422,579.85	$467,390,224.98	$150,016,739.64	$150,016,739.64	-$60,006,695.86	$90,010,043.78
2032	100%					-$125,644,452.66	-$200,255,257.24	$481,411,931.73	$155,512,221.83	$155,512,221.83	-$62,204,888.73	$93,307,333.10
2033	100%					-$129,413,786.24	-$206,262,914.96	$495,854,289.68	$160,177,588.48	$160,177,588.48	-$64,071,035.39	$96,106,553.09
2034	100%					-$133,296,199.83	-$212,450,802.41	$510,729,918.37	$164,982,916.14	$164,982,916.14	-$65,993,166.46	$98,989,749.68
2035	100%					-$137,295,085.82	-$218,824,326.48	$526,051,815.92	$169,932,403.62	$169,932,403.62	-$67,972,961.45	$101,959,442.17
2036	100%		-$966,000.00			-$141,413,938.39	-$225,389,056.28	$541,833,370.40	$174,064,375.73	$174,064,375.73	-$69,625,750.29	$104,438,625.44
2037	100%					-$145,656,356.55	-$232,150,727.96	$558,088,371.51	$180,281,287.00	$180,281,287.00	-$72,112,514.80	$108,168,772.20
2038	100%					-$150,026,047.24	-$239,115,249.80	$574,831,022.66	$185,689,725.61	$185,689,725.61	-$74,275,890.25	$111,413,835.37
2039	100%					-$154,526,828.66	-$246,288,707.30	$592,075,953.34	$191,260,417.38	$191,260,417.38	-$76,504,166.95	$114,756,250.43
2040	100%					-$159,162,633.52	-$253,677,368.52	$609,838,231.94	$196,998,229.90	$196,998,229.90	-$78,799,291.96	$118,198,937.94

Year	Plant Capacity	Total Capital Investment	Catalyst Charge	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2041	100%		-$966,000.00			-$163,937,512.53	-$261,287,689.57	$628,133,378.90	$201,942,176.80	$201,942,176.80	-$80,776,870.72	$121,165,306.08
2042	100%					-$168,855,637.90	-$269,126,320.26	$646,977,380.26	$208,995,422.10	$208,995,422.10	-$83,598,168.84	$125,397,253.26
2043	100%					-$173,921,307.04	-$277,200,109.87	$666,386,701.67	$215,265,284.77	$215,265,284.77	-$86,106,113.91	$129,159,170.86
2044	100%					-$179,138,946.25	-$285,516,113.16	$686,378,302.72	$221,723,243.31	$221,723,243.31	-$88,689,297.32	$133,033,945.99
2045	100%					-$184,513,114.64	-$294,081,596.56	$706,969,651.80	$228,374,940.61	$228,374,940.61	-$91,349,976.24	$137,024,964.37
2046	100%		-$966,000.00			-$190,048,508.08	-$302,904,044.45	$728,178,741.36	$234,260,188.83	$234,260,188.83	-$93,704,075.53	$140,556,113.30
2047	100%					-$195,749,963.32	-$311,991,165.79	$750,024,103.60	$242,282,974.49	$242,282,974.49	-$96,913,189.80	$145,369,784.70
2048	100%					-$201,622,462.22	-$321,350,900.76	$772,524,826.71	$249,551,463.73	$249,551,463.73	-$99,820,585.49	$149,730,878.24
2049	100%					-$207,671,136.08	-$330,991,427.78	$795,700,571.51	$257,038,007.64	$257,038,007.64	-$102,815,203.06	$154,222,804.58
2050	100%					-$213,901,270.17	-$340,921,170.62	$819,571,588.65	$264,749,147.87	$264,749,147.87	-$105,899,659.15	$158,849,488.72
											Net Present Value	**-$48,174,085.70**
											IRR	**13.84%**

Economics Spreadsheets Step 1

Total Capital Investment

Total Cost Fabricated Equipment and Process Machinery	**$202,478,956.77**
Cost of Spares	$40,495,791.35
Initial Catalyst Charge	$996,000.00
Cost for Computers and software	$10,000,000.00
Total Bare Module Investment	**$253,970,748.12**
Site Preparation	$12,148,737.41
Service Facilities	$10,123,947.84
Allocated costs for Utilities:	
Steam	$15,782,076.20
Electricity	$574,989.42
Cooling Water	$468,127.85
Process Water	$29,829.74
Refrigeration	$5,614,720.23
Total Allocated Costs for Utilities and Related Facilities	$22,469,743.43
Direct Permanent Investment	**$298,713,176.79**
Cost of Contingencies and Contractors Fees	**$104,549,611.88**
Total Depreciable Capital	**$403,262,788.67**
Land	$8,065,255.77
Initial Royalty Fee	$8,065,255.77
Cost for Start-up	$40,326,278.87
Site Factor - Gulf Coast	1
Total Permanent Investment	**$459,719,579.08**
Working Capital:	
Cash Reserves - 1 Month	$5,622,937.27
Inventories for Products - 1 Week	$2,935,254.81
Accounts Receivable	$12,719,437.50
Accounts Payable	$6,302,828.42
Total Working Capital	**$27,580,458.00**
Total Capital Investment	**$487,300,037.08**

Utilities

Name	Fluid	Rate	Rate Units	Cost	Units	Cost per Hour	Cost Units	Total Yearly Cost
Electricity		162.355	KW	$0.06	USD/KW-H	$9.74	USD/H	$81,826.92
Cooling Water	Water	507175	GAL/H	$0.08	USD/1000gal	$38.04	USD/H	$319,520.25
Process Water Start Up	Water	22525	GAL	$0.75	USD/1000gal	$16.89	USD	$16.89
Process Water	Water	22.525	GAL/H	$0.75	USD/1000gal	$0.02	USD/H	$141.91
Refrigerant - Propane	Refrigerant	261.3359	KLB/H	$0.07	USD/Ton-H	$9.26	USD/H	$77,747.43
Refrigerant - Freon 12	Refrigerant	1064.454	KLB/H	$0.10	USD/Ton-H	$53.22	USD/H	$447,070.68
Steam @100PSI	Steam	108.3391	KLB/H	$4.14	USD/1000lbs	$448.52	USD/H	$3,767,600.54
Steam @165PSI	Steam	86.3409	KLB/H	$4.96	USD/1000lbs	$428.25	USD/H	$3,597,307.26
Steam @400PSI	Steam	20.97	KLB/H	$6.41	USD/1000lbs	$134.35	USD/H	$1,128,547.74
							Total Utility Costs	**$9,890,768.60**

Total Fixed Costs

Utilities	**Total Utility Costs**	**$9,890,768.60**
Labor-related Operations	Days of Operation	350
	Hours of operation per year	8400
	Hours of operation per week	168
	Operator hours per week	40
	Operators shifts per week	4.2
	due to sickness/vacation, assume:	5
	Number of sections	1
	Operators per section table 23.3	1
	Total operators per shift	1
	Hours per shift	8
	Weeks of operation	50
	Wage	$35.00
	Texas/Gulf cost factor	1
	Direct wages & benefits	$350,000.00
	Direct salaries & benefits	$52,500.00
	Operating supplies and services	$21,000.00
	Technical assistance to manufacturing	$300,000.00
	Control laboratory	$325,000.00
	Total Operations Annual Cost, O	**$1,048,500.00**
Maintenance	Total Depreciable Capital - from TCI page	$403,262,788.67
	Maintenance wage & benefits	$16,937,037.12
	Salaries & benefits	$5,081,111.14
	Materials & services	$20,324,444.55
	Maintenance overhead	$1,016,222.23
	Total Annual Maintenance Costs, M	**$43,358,815.04**
Operating Overhead	DW&B	$350,000.00
	Direct salaries and benefits	$52,500.00
	MW&B	$16,937,037.12
	Maintenance salaries and benefits	$5,081,111.14
	Total Annual M&O-SW&B	**$22,420,648.26**
	General plant overhead	$1,591,866.03

	Mechanical department services	$538,095.56
	Employee relations department	$1,322,818.25
	Business services	$1,659,127.97
	Total Annual Operating Overhead, O	**$5,111,907.80**
Property Taxes & Insurance	**Total Property Taxes & Insurance**	**$8,065,255.77**
Depreciation	Please see MACRS depreciation in Cash Flow (not included in COM)	
	Total Cost of Manufacture, COM	**$67,475,247.22**
	Total Fixed Costs	**$67,475,247.22**

Total Variable Costs and Total Variable Revenues

	Name	**Cost**	**Unit**	**lbs/yr**	**Total Cost**
Raw Materials	Ethylene	$0.46	USD/lb	150494400	$69,227,424.00
	Oxygen	$0.05	USD/lb	123916800	$6,195,840.00
	CO2 Removal solvents/MEA	$0.31	USD/barrel EO	679603.428	$210,677.06
				Cost of Raw Materials	**$75,633,941.06**
Product Sales	Ethylene Oxide	$0.75	USD/lb	203511000	$152,633,250.00
General Expenses	Selling/Transfer expense	3%			
	Direct Research	4.8%			
	Allocated Research	0.5%			
	Administrative Expenses	2%			
	Management incentive compensation	1.25%			
	Total General Expenses as a function of Revenues	12%			$18,315,990.00
Total Variable Costs					**$93,949,931.06**
Total Variable Revenues					**$152,633,250.00**

Cash Flow

Year	Plant Capacity	Total Capital Investment	Catalyst Charge	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2015	0%	-$487,300,037.08							-$487,300,037.08	$0.00	$0.00	-$487,300,037.08
2016	50%			0.2	-$80,652,557.73	-$67,475,247.22	-$46,974,965.53	$76,316,625.00	-$38,133,587.75	-$118,786,145.48	$0.00	-$38,133,587.75
2017	100%			0.32	-$129,044,092.37	-$69,499,504.63	-$96,768,428.99	$157,212,247.50	-$9,055,686.13	-$138,099,778.50	$0.00	-$9,055,686.13
2018	100%			0.192	-$77,426,455.42	-$71,584,489.77	-$99,671,481.86	$161,928,614.93	-$9,327,356.71	-$86,753,812.14	$0.00	-$9,327,356.71
2019	100%			0.1152	-$46,455,873.25	-$73,732,024.46	-$102,661,626.32	$166,786,473.37	-$9,607,177.41	-$56,063,050.67	$0.00	-$9,607,177.41
2020	100%			0.1152	-$46,455,873.25	-$75,943,985.20	-$105,741,475.11	$171,790,067.57	-$9,895,392.73	-$56,351,265.99	$0.00	-$9,895,392.73
2021	100%		-$966,000.00	0.0576	-$23,227,936.63	-$78,222,304.75	-$108,913,719.36	$176,943,769.60	-$11,158,254.52	-$34,386,191.14	$0.00	-$11,158,254.52
2022	100%					-$80,568,973.90	-$112,181,130.94	$182,252,082.69	-$10,498,022.15	-$10,498,022.15	$0.00	-$10,498,022.15
2023	100%					-$82,986,043.11	-$115,546,564.87	$187,719,645.17	-$10,812,962.82	-$10,812,962.82	$0.00	-$10,812,962.82
2024	100%					-$85,475,624.41	-$119,012,961.82	$193,351,234.52	-$11,137,351.70	-$11,137,351.70	$0.00	-$11,137,351.70
2025	100%					-$88,039,893.14	-$122,583,350.67	$199,151,771.56	-$11,471,472.25	-$11,471,472.25	$0.00	-$11,471,472.25
2026	100%		-$966,000.00			-$90,681,089.93	-$126,260,851.19	$205,126,324.71	-$12,781,616.42	-$12,781,616.42	$0.00	-$12,781,616.42
2027	100%					-$93,401,522.63	-$130,048,676.73	$211,280,114.45	-$12,170,084.91	-$12,170,084.91	$0.00	-$12,170,084.91
2028	100%					-$96,203,568.31	-$133,950,137.03	$217,618,517.88	-$12,535,187.46	-$12,535,187.46	$0.00	-$12,535,187.46
2029	100%					-$99,089,675.36	-$137,968,641.14	$224,147,073.42	-$12,911,243.08	-$12,911,243.08	$0.00	-$12,911,243.08
2030	100%					-$102,062,365.62	-$142,107,700.38	$230,871,485.62	-$13,298,580.38	-$13,298,580.38	$0.00	-$13,298,580.38
2031	100%		-$966,000.00			-$105,124,236.59	-$146,370,931.39	$237,797,630.19	-$14,663,537.79	-$14,663,537.79	$0.00	-$14,663,537.79
2032	100%					-$108,277,963.69	-$150,762,059.33	$244,931,559.10	-$14,108,463.92	-$14,108,463.92	$0.00	-$14,108,463.92
2033	100%					-$111,526,302.60	-$155,284,921.11	$252,279,505.87	-$14,531,717.84	-$14,531,717.84	$0.00	-$14,531,717.84
2034	100%					-$114,872,091.68	-$159,943,468.74	$259,847,891.04	-$14,967,669.37	-$14,967,669.37	$0.00	-$14,967,669.37
2035	100%					-$118,318,254.43	-$164,741,772.80	$267,643,327.78	-$15,416,699.45	-$15,416,699.45	$0.00	-$15,416,699.45
2036	100%		-$966,000.00			-$121,867,802.06	-$169,684,025.99	$275,672,627.61	-$16,845,200.44	-$16,845,200.44	$0.00	-$16,845,200.44
2037	100%					-$125,523,836.12	-$174,774,546.77	$283,942,806.44	-$16,355,576.45	-$16,355,576.45	$0.00	-$16,355,576.45
2038	100%					-$129,289,551.20	-$180,017,783.17	$292,461,090.63	-$16,846,243.74	-$16,846,243.74	$0.00	-$16,846,243.74
2039	100%					-$133,168,237.74	-$185,418,316.67	$301,234,923.35	-$17,351,631.06	-$17,351,631.06	$0.00	-$17,351,631.06
2040	100%					-$137,163,284.87	-$190,980,866.17	$310,271,971.05	-$17,872,179.99	-$17,872,179.99	$0.00	-$17,872,179.99

Year	Plant Capacity	Total Capital Investment	Catalyst Charge	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2041	100%		-$966,000.00			-$141,278,183.42	-$196,710,292.15	$319,580,130.18	-$19,374,345.39	-$19,374,345.39	$0.00	-$19,374,345.39
2042	100%					-$145,516,528.92	-$202,611,600.92	$329,167,534.09	-$18,960,595.75	-$18,960,595.75	$0.00	-$18,960,595.75
2043	100%					-$149,882,024.79	-$208,689,948.94	$339,042,560.11	-$19,529,413.62	-$19,529,413.62	$0.00	-$19,529,413.62
2044	100%					-$154,378,485.53	-$214,950,647.41	$349,213,836.91	-$20,115,296.03	-$20,115,296.03	$0.00	-$20,115,296.03
2045	100%					-$159,009,840.10	-$221,399,166.83	$359,690,252.02	-$20,718,754.91	-$20,718,754.91	$0.00	-$20,718,754.91
2046	100%		-$966,000.00			-$163,780,135.30	-$228,041,141.84	$370,480,959.58	-$22,306,317.56	-$22,306,317.56	$0.00	-$22,306,317.56
2047	100%					-$168,693,539.36	-$234,882,376.09	$381,595,388.37	-$21,980,527.09	-$21,980,527.09	$0.00	-$21,980,527.09
2048	100%					-$173,754,345.54	-$241,928,847.38	$393,043,250.02	-$22,639,942.90	-$22,639,942.90	$0.00	-$22,639,942.90
2049	100%					-$178,966,975.91	-$249,186,712.80	$404,834,547.52	-$23,319,141.19	-$23,319,141.19	$0.00	-$23,319,141.19
2050	100%					-$184,335,985.18	-$256,662,314.18	$416,979,583.95	-$24,018,715.42	-$24,018,715.42	$0.00	-$24,018,715.42
											Net Present Value	**-$585,350,578.54**

Economics Spreadsheets Step 2

Total Capital Investment

Total Cost Fabricated Equipment and Process Machinery	**$20,828,257.19**
Cost of Spares	$4,165,651.44
Initial Catalyst Charge	$996,000.00
Cost for Computers and software	$10,000,000.00
Total Bare Module Investment	**$35,989,908.62**
Site Preparation	$1,249,695.43
Service Facilities	$1,041,412.86
Allocated costs for Utilities:	
Steam	$760,410.65
Electricity	$2,378,411.66
Cooling Water	$589,928.46
Process Water	$0.00
Refrigeration	$225,808.00
Total Allocated Costs for Utilities and Related Facilities	**$3,954,558.77**
Direct Permanent Investment	**$42,235,575.69**
Cost of Contingencies and Contractors Fees	**$14,782,451.49**
Total Depreciable Capital	**$57,018,027.18**
Land	$1,140,360.54
Initial Royalty Fee	$1,140,360.54
Cost for Start-up	$5,701,802.72
Site Factor - Gulf Coast	1
Total Permanent Investment	**$65,000,550.98**
Working Capital:	
Cash Reserves - 1 Month	$869,214.77
Inventories for Products - 1 Week	$5,130,242.41
Accounts Receivable	$22,231,050.45
Accounts Payable	$13,773,980.39
Total Working Capital	**$42,004,488.02**
Total Capital Investment	**$107,005,039.00**

Utilities

Name	Fluid	Rate	Rate Units	Cost	Units	Cost per Hour	Cost Units	Total Yearly Cost
Electricity		898.235	KW	$0.06	USD/KW-H	$53.89	USD/H	$452,710.44
Cooling Water	Water	712617	GAL/H	$0.08	USD/1000gal	$53.45	USD/H	$448,948.71
Refrigerant - Propane	Refrigerant	4.74008	KLB/H	$0.07	USD/Ton-H	$0.17	USD/H	$1,410.17
Refrigerant - Freon 12	Refrigerant	48.5794	KLB/H	$0.10	USD/Ton-H	$2.43	USD/H	$20,403.35
Steam @100PSI	Steam	4.60524	KLB/H	$4.14	USD/1000lbs	$19.07	USD/H	$160,151.83
							Total Utility Costs (CE index adjusted)	**$1,137,805.72**

Total Fixed Costs

Utilities	**Total Utility Costs**	**$1,137,805.72**
Labor-related Operations	Days of Operation	350
	Hours of operation per year	8400
	Hours of operation per week	168
	Operator hours per week	40
	Operators shifts per week	4.2
	due to sickness/vacation, assume:	5
	Total operators per shift	1.333333333
	Hours per shift	8
	Weeks of operation	50
	Wage	$35.00
	Texas/Gulf cost factor	1
	Direct wages & benefits	$466,666.67
	Direct salaries & benefits	$70,000.00
	Operating supplies and services	$28,000.00
	Technical assistance to manufacturing	$300,000.00
	Control laboratory	$325,000.00
	Total Operations Annual Cost, O	**$1,189,666.67**
Maintenance	Total Depreciable Capital - from TCI page	$57,018,027.18
	Maintenance wage & benefits	$2,394,757.14
	Salaries & benefits	$718,427.14
	Materials & services	$2,873,708.57
	Maintenance overhead	$143,685.43
	Total Annual Maintenance Costs, M	**$6,130,578.28**
Operating Overhead	DW&B	$466,666.67
	Direct salaries and benefits	$70,000.00
	MW&B	$2,394,757.14
	Maintenance salaries and benefits	$718,427.14
	Total Annual M&O-SW&B	**$3,649,850.95**
	General plant overhead	$259,139.42
	Mechanical department services	$87,596.42
	Employee relations department	$215,341.21
	Business services	$270,088.97

	Total Annual Operating Overhead, O	**$832,166.02**
Property Taxes & Insurance	**Total Property Taxes & Insurance**	**$1,140,360.54**
Depreciation	Please see MACRS depreciation in Cash Flow (not in COM)	
	Total Cost of Manufacture, COM	**$10,430,577.23**
	Total Fixed Costs	**$10,430,577.23**

Total Variable Costs and Total Variable Revenues

	Name	Cost	Unit	lbs/yr	Total Cost
Raw Materials	Ethylene Oxide	$0.75	USD/lb	203511000	$152,633,250.00
	Carbon Monoxide	$0.10	USD/lb	126545146.6	$12,654,514.66
				Cost of Raw Materials	**$165,287,764.66**
Product Sales	β-Propiolactone	$0.85	USD/lb	313850124	$266,772,605.40
General Expenses	Selling/Transfer expense	3%			
	Direct Research	4.8%			
	Allocated Research	0.5%			
	Administrative Expenses	2%			
	Management incentive compensation	1.25%			
	Total General Expenses as a function of Revenues	12%			$32,012,712.65
Total Variable Costs					**$197,300,477.30**
Total Variable Revenues					**$266,772,605.40**

Cash Flow

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2015	0%	-$107,005,039.00						-$107,005,039.00	$0.00	$0.00	-$107,005,039.00
2016	50%		0.2	-$11,403,605.44	-$10,430,577.23	-$98,650,238.65	$133,386,302.70	$24,305,486.82	$12,901,881.38	-$5,160,752.55	$19,144,734.26
2017	100%		0.32	-$18,245,768.70	-$10,743,494.55	-$203,219,491.62	$274,775,783.56	$60,812,797.39	$42,567,028.69	-$17,026,811.48	$43,785,985.91
2018	100%		0.192	-$10,947,461.22	-$11,065,799.39	-$209,316,076.37	$283,019,057.07	$62,637,181.31	$51,689,720.09	-$20,675,888.04	$41,961,293.27
2019	100%		0.1152	-$6,568,476.73	-$11,397,773.37	-$215,595,558.66	$291,509,628.78	$64,516,296.75	$57,947,820.02	-$23,179,128.01	$41,337,168.74
2020	100%		0.1152	-$6,568,476.73	-$11,739,706.57	-$222,063,425.42	$300,254,917.64	$66,451,785.65	$59,883,308.92	-$23,953,323.57	$42,498,462.08
2021	100%		0.0576	-$3,284,238.37	-$12,091,897.77	-$228,725,328.19	$309,262,565.17	$68,445,339.22	$65,161,100.86	-$26,064,440.34	$42,380,898.88
2022	100%				-$12,454,654.70	-$235,587,088.03	$318,540,442.13	$70,498,699.40	$70,498,699.40	-$28,199,479.76	$42,299,219.64
2023	100%				-$12,828,294.34	-$242,654,700.67	$328,096,655.39	$72,613,660.38	$72,613,660.38	-$29,045,464.15	$43,568,196.23
2024	100%				-$13,213,143.17	-$249,934,341.69	$337,939,555.05	$74,792,070.19	$74,792,070.19	-$29,916,828.08	$44,875,242.12
2025	100%				-$13,609,537.46	-$257,432,371.94	$348,077,741.71	$77,035,832.30	$77,035,832.30	-$30,814,332.92	$46,221,499.38
2026	100%				-$14,017,823.59	-$265,155,343.10	$358,520,073.96	$79,346,907.27	$79,346,907.27	-$31,738,762.91	$47,608,144.36
2027	100%				-$14,438,358.30	-$273,110,003.39	$369,275,676.18	$81,727,314.49	$81,727,314.49	-$32,690,925.79	$49,036,388.69
2028	100%				-$14,871,509.04	-$281,303,303.50	$380,353,946.46	$84,179,133.92	$84,179,133.92	-$33,671,653.57	$50,507,480.35
2029	100%				-$15,317,654.32	-$289,742,402.60	$391,764,564.86	$86,704,507.94	$86,704,507.94	-$34,681,803.18	$52,022,704.76
2030	100%				-$15,777,183.95	-$298,434,674.68	$403,517,501.80	$89,305,643.18	$89,305,643.18	-$35,722,257.27	$53,583,385.91
2031	100%				-$16,250,499.46	-$307,387,714.92	$415,623,026.85	$91,984,812.47	$91,984,812.47	-$36,793,924.99	$55,190,887.48
2032	100%				-$16,738,014.45	-$316,609,346.37	$428,091,717.66	$94,744,356.85	$94,744,356.85	-$37,897,742.74	$56,846,614.11
2033	100%				-$17,240,154.88	-$326,107,626.76	$440,934,469.19	$97,586,687.55	$97,586,687.55	-$39,034,675.02	$58,552,012.53
2034	100%				-$17,757,359.53	-$335,890,855.56	$454,162,503.27	$100,514,288.18	$100,514,288.18	-$40,205,715.27	$60,308,572.91
2035	100%				-$18,290,080.31	-$345,967,581.23	$467,787,378.36	$103,529,716.82	$103,529,716.82	-$41,411,886.73	$62,117,830.09
2036	100%				-$18,838,782.72	-$356,346,608.66	$481,820,999.71	$106,635,608.33	$106,635,608.33	-$42,654,243.33	$63,981,365.00
2037	100%				-$19,403,946.20	-$367,037,006.92	$496,275,629.71	$109,834,676.58	$109,834,676.58	-$43,933,870.63	$65,900,805.95
2038	100%				-$19,986,064.59	-$378,048,117.13	$511,163,898.60	$113,129,716.87	$113,129,716.87	-$45,251,886.75	$67,877,830.12
2039	100%				-$20,585,646.53	-$389,389,560.65	$526,498,815.56	$116,523,608.38	$116,523,608.38	-$46,609,443.35	$69,914,165.03
2040	100%				-$21,203,215.92	-$401,071,247.47	$542,293,780.02	$120,019,316.63	$120,019,316.63	-$48,007,726.65	$72,011,589.98

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2041	100%				-$21,839,312.40	-$413,103,384.89	$558,562,593.42	$123,619,896.13	$123,619,896.13	-$49,447,958.45	$74,171,937.68
2042	100%				-$22,494,491.77	-$425,496,486.44	$575,319,471.23	$127,328,493.02	$127,328,493.02	-$50,931,397.21	$76,397,095.81
2043	100%				-$23,169,326.53	-$438,261,381.03	$592,579,055.36	$131,148,347.81	$131,148,347.81	-$52,459,339.12	$78,689,008.68
2044	100%				-$23,864,406.32	-$451,409,222.46	$610,356,427.02	$135,082,798.24	$135,082,798.24	-$54,033,119.30	$81,049,678.94
2045	100%				-$24,580,338.51	-$464,951,499.13	$628,667,119.83	$139,135,282.19	$139,135,282.19	-$55,654,112.87	$83,481,169.31
2046	100%				-$25,317,748.67	-$478,900,044.11	$647,527,133.43	$143,309,340.65	$143,309,340.65	-$57,323,736.26	$85,985,604.39
2047	100%				-$26,077,281.13	-$493,267,045.43	$666,952,947.43	$147,608,620.87	$147,608,620.87	-$59,043,448.35	$88,565,172.52
2048	100%				-$26,859,599.56	-$508,065,056.79	$686,961,535.85	$152,036,879.50	$152,036,879.50	-$60,814,751.80	$91,222,127.70
2049	100%				-$27,665,387.55	-$523,307,008.50	$707,570,381.93	$156,597,985.88	$156,597,985.88	-$62,639,194.35	$93,958,791.53
2050	100%				-$28,495,349.18	-$539,006,218.75	$728,797,493.39	$161,295,925.46	$161,295,925.46	-$64,518,370.18	$96,777,555.28
										Net Present Value	**$179,582,851.13**
										IRR	**34.72%**

Economics Spreadsheets Step 3

Total Capital Investment

Total Cost Fabricated Equipment and Process Machinery	**$2,768,483.15**
Cost of Spares	$553,696.63
Initial Catalyst Charge	$996,000.00
Cost for Computers and software	$10,000,000.00
Total Bare Module Investment	**$14,318,179.78**
Site Preparation	$166,108.99
Service Facilities	$138,424.16
Allocated costs for Utilities:	
Steam	$2,570,745.94
Electricity	$321,762.49
Cooling Water	$321,808.50
Process Water	$0.00
Refrigeration	$0.00
Total Allocated Costs for Utilities and Related Facilities	$3,214,316.93
Direct Permanent Investment	**$17,837,029.86**
Cost of Contingencies and Contractors Fees	**$6,242,960.45**
Total Depreciable Capital	**$24,079,990.31**
Land	$481,599.81
Initial Royalty Fee	$481,599.81
Cost for Start-up	$2,407,999.03
Site Factor - Gulf Coast	1
Total Permanent Investment	**$27,451,188.95**
Working Capital:	
Cash Reserves - 1 Month	$507,486.13
Inventories for Products - 1 Week	$5,769,230.77
Accounts Receivable	$25,000,000.00
Accounts Payable	$22,273,050.45
Total Working Capital	**$53,549,767.35**
Total Capital Investment	**$81,000,956.30**

Utilities

Name	Fluid	Rate	Rate Units	Cost	Units	Cost per Hour	Cost Units	Total Yearly Cost
Electricity		80.668	KW	$0.06	USD/KW-H	$4.84	USD/H	$40,656.67
Cooling Water	Water	292277	GAL/H	$0.08	USD/1000gal	$21.92	USD/H	$184,134.51
Steam @400PSI	Steam	20.71821	KLB/H	$6.41	USD/1000lbs	$132.80	USD/H	$1,115,551.30
						Total Utility Costs		**$1,407,359.61**

Total Fixed Costs

Utilities	**Total Utility Costs**	**$1,407,359.61**
Labor-related Operations	Days of Operation	350
	Hours of operation per year	8400
	Hours of operation per week	168
	Operator hours per week	40
	Operators shifts per week	4.2
	due to sickness/vacation, assume:	5
	Total operators per shift	1.333333333
	Hours per shift	8
	Weeks of operation	50
	Wage	$35.00
	Texas/Gulf cost factor	1
	Direct wages & benefits	$466,666.67
	Direct salaries & benefits	$70,000.00
	Operating supplies and services	$28,000.00
	Technical assistance to manufacturing	$300,000.00
	Control laboratory	$325,000.00
	Total Operations Annual Cost, O	**$1,189,666.67**
Maintenance	Total Depreciable Capital - from TCI page	$24,079,990.31
	Maintenance wage & benefits	$1,011,359.59
	Salaries & benefits	$303,407.88
	Materials & services	$1,213,631.51
	Maintenance overhead	$60,681.58
	Total Annual Maintenance Costs, M	**$2,589,080.56**
Operating Overhead	DW&B	$466,666.67
	Direct salaries and benefits	$70,000.00
	MW&B	$1,011,359.59
	Maintenance salaries and benefits	$303,407.88
	Total Annual M&O-SW&B	**$1,851,434.14**
	General plant overhead	$131,451.82
	Mechanical department services	$44,434.42
	Employee relations department	$109,234.61
	Business services	$137,006.13

	Total Annual Operating Overhead, O	**$422,126.98**
Property Taxes & Insurance	**Total Property Taxes & Insurance**	**$481,599.81**
Depreciation	Please see MACRS depreciation in Cash Flow (not in COM)	
	Total Cost of Manufacture, COM	**$6,089,833.62**
	Total Fixed Costs	**$6,089,833.62**

Total Variable Costs and Total Variable Revenues

	Name	**Cost**	**Unit**	**lbs/yr**	**Total Cost**
Raw Materials	β-Propiolactone	$0.85	USD/lb	313850124	$266,772,605.40
	MEHQ	$5.00	USD/lb	100800	$504,000.00
				Cost of Raw Materials	**$267,276,605.40**
Product Sales	Acrylic Acid	$1.00	USD/lb	300000000	$300,000,000.00
General Expenses	Selling/Transfer expense	3%			
	Direct Research	4.8%			
	Allocated Research	0.5%			
	Administrative Expenses	2%			
	Management incentive compensation	1.25%			
	Total General Expenses as a function of Revenues	12%			$36,000,000.00
				Total Variable Costs	**$303,276,605.40**
				Total Variable Revenues	**$300,000,000.00**

Cash Flow

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2015	0%	-$81,000,956.30						-$81,000,956.30	$0.00	$0.00	-$81,000,956.30
2016	50%		0.2	-$4,815,998.06	-$6,089,833.62	-$151,638,302.70	$150,000,000.00	-$7,728,136.32	-$12,544,134.38	$0.00	-$7,728,136.32
2017	100%		0.32	-$7,705,596.90	-$6,272,528.63	-$312,374,903.56	$309,000,000.00	-$9,647,432.19	-$17,353,029.09	$0.00	-$9,647,432.19
2018	100%		0.192	-$4,623,358.14	-$6,460,704.49	-$321,746,150.67	$318,270,000.00	-$9,936,855.16	-$14,560,213.29	$0.00	-$9,936,855.16
2019	100%		0.1152	-$2,774,014.88	-$6,654,525.62	-$331,398,535.19	$327,818,100.00	-$10,234,960.81	-$13,008,975.69	$0.00	-$10,234,960.81
2020	100%		0.1152	-$2,774,014.88	-$6,854,161.39	-$341,340,491.24	$337,652,643.00	-$10,542,009.63	-$13,316,024.52	$0.00	-$10,542,009.63
2021	100%		0.0576	-$1,387,007.44	-$7,059,786.23	-$351,580,705.98	$347,782,222.29	-$10,858,269.92	-$12,245,277.37	$0.00	-$10,858,269.92
2022	100%				-$7,271,579.82	-$362,128,127.16	$358,215,688.96	-$11,184,018.02	-$11,184,018.02	$0.00	-$11,184,018.02
2023	100%				-$7,489,727.21	-$372,991,970.98	$368,962,159.63	-$11,519,538.56	-$11,519,538.56	$0.00	-$11,519,538.56
2024	100%				-$7,714,419.03	-$384,181,730.11	$380,031,024.42	-$11,865,124.72	-$11,865,124.72	$0.00	-$11,865,124.72
2025	100%				-$7,945,851.60	-$395,707,182.01	$391,431,955.15	-$12,221,078.46	-$12,221,078.46	$0.00	-$12,221,078.46
2026	100%				-$8,184,227.15	-$407,578,397.47	$403,174,913.80	-$12,587,710.81	-$12,587,710.81	$0.00	-$12,587,710.81
2027	100%				-$8,429,753.96	-$419,805,749.39	$415,270,161.22	-$12,965,342.14	-$12,965,342.14	$0.00	-$12,965,342.14
2028	100%				-$8,682,646.58	-$432,399,921.87	$427,728,266.05	-$13,354,302.40	-$13,354,302.40	$0.00	-$13,354,302.40
2029	100%				-$8,943,125.98	-$445,371,919.53	$440,560,114.04	-$13,754,931.47	-$13,754,931.47	$0.00	-$13,754,931.47
2030	100%				-$9,211,419.76	-$458,733,077.12	$453,776,917.46	-$14,167,579.42	-$14,167,579.42	$0.00	-$14,167,579.42
2031	100%				-$9,487,762.35	-$472,495,069.43	$467,390,224.98	-$14,592,606.80	-$14,592,606.80	$0.00	-$14,592,606.80
2032	100%				-$9,772,395.22	-$486,669,921.51	$481,411,931.73	-$15,030,385.01	-$15,030,385.01	$0.00	-$15,030,385.01
2033	100%				-$10,065,567.08	-$501,270,019.16	$495,854,289.68	-$15,481,296.56	-$15,481,296.56	$0.00	-$15,481,296.56
2034	100%				-$10,367,534.09	-$516,308,119.73	$510,729,918.37	-$15,945,735.45	-$15,945,735.45	$0.00	-$15,945,735.45
2035	100%				-$10,678,560.11	-$531,797,363.33	$526,051,815.92	-$16,424,107.52	-$16,424,107.52	$0.00	-$16,424,107.52
2036	100%				-$10,998,916.92	-$547,751,284.23	$541,833,370.40	-$16,916,830.74	-$16,916,830.74	$0.00	-$16,916,830.74
2037	100%				-$11,328,884.42	-$564,183,822.75	$558,088,371.51	-$17,424,335.66	-$17,424,335.66	$0.00	-$17,424,335.66
2038	100%				-$11,668,750.96	-$581,109,337.43	$574,831,022.66	-$17,947,065.73	-$17,947,065.73	$0.00	-$17,947,065.73
2039	100%				-$12,018,813.49	-$598,542,617.56	$592,075,953.34	-$18,485,477.71	-$18,485,477.71	$0.00	-$18,485,477.71
2040	100%				-$12,379,377.89	-$616,498,896.08	$609,838,231.94	-$19,040,042.04	-$19,040,042.04	$0.00	-$19,040,042.04

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2041	100%				-$12,750,759.23	-$634,993,862.97	$628,133,378.90	-$19,611,243.30	-$19,611,243.30	$0.00	-$19,611,243.30
2042	100%				-$13,133,282.00	-$654,043,678.86	$646,977,380.26	-$20,199,580.60	-$20,199,580.60	$0.00	-$20,199,580.60
2043	100%				-$13,527,280.46	-$673,664,989.22	$666,386,701.67	-$20,805,568.01	-$20,805,568.01	$0.00	-$20,805,568.01
2044	100%				-$13,933,098.88	-$693,874,938.90	$686,378,302.72	-$21,429,735.06	-$21,429,735.06	$0.00	-$21,429,735.06
2045	100%				-$14,351,091.84	-$714,691,187.07	$706,969,651.80	-$22,072,627.11	-$22,072,627.11	$0.00	-$22,072,627.11
2046	100%				-$14,781,624.60	-$736,131,922.68	$728,178,741.36	-$22,734,805.92	-$22,734,805.92	$0.00	-$22,734,805.92
2047	100%				-$15,225,073.34	-$758,215,880.36	$750,024,103.60	-$23,416,850.10	-$23,416,850.10	$0.00	-$23,416,850.10
2048	100%				-$15,681,825.54	-$780,962,356.77	$772,524,826.71	-$24,119,355.60	-$24,119,355.60	$0.00	-$24,119,355.60
2049	100%				-$16,152,280.30	-$804,391,227.47	$795,700,571.51	-$24,842,936.27	-$24,842,936.27	$0.00	-$24,842,936.27
2050	100%				-$16,636,848.71	-$828,522,964.30	$819,571,588.65	-$25,588,224.36	-$25,588,224.36	$0.00	-$25,588,224.36
										Net Present Value	**-$155,980,809.87**

Economics Spreadsheets 2-Step Process

Total Capital Investment

Total Cost Fabricated Equipment and Process Machinery	**$23,596,740.33**
Cost of Spares	$4,719,348.07
Initial Catalyst Charge	$996,000.00
Cost for Computers and software	$10,000,000.00
Total Bare Module Investment	**$39,312,088.40**
Site Preparation	$1,415,804.42
Service Facilities	$1,179,837.02
Allocated costs for Utilities:	
Steam	$3,024,596.04
Electricity	$2,554,390.35
Cooling Water	$745,244.74
Process Water	$0.00
Refrigeration	$225,808.00
Total Allocated Costs for Utilities and Related Facilities	**$6,550,039.13**
Direct Permanent Investment	**$48,457,768.97**
Cost of Contingencies and Contractors Fees	**$16,960,219.14**
Total Depreciable Capital	**$65,417,988.11**
Land	$1,308,359.76
Initial Royalty Fee	$1,308,359.76
Cost for Start-up	$6,541,798.81
Site Factor - Gulf Coast	1
Total Permanent Investment	**$74,576,506.45**
Working Capital:	
Cash Reserves - 1 Month	$1,113,098.55
Inventories for Products - 1 Week	$5,769,230.77
Accounts Receivable	$25,000,000.00
Accounts Payable	$13,815,980.39
Total Working Capital	**$45,698,309.71**
Total Capital Investment	**$120,274,816.16**

Utilities

	Name	Fluid	Rate	Rate Units	Cost	Units	Cost per Hour	Cost Units	Total Yearly Cost
STEP 2	Electricity		898.235	KW	$0.06	USD/KW-H	$53.89	USD/H	$452,710.44
	Cooling Water	Water	712617	GAL/H	$0.08	USD/1000gal	$53.45	USD/H	$448,948.71
	Refrigerant - Propane	Refrigerant	4.74008	KLB/H	$0.07	USD/Ton-H	$0.17	USD/H	$1,410.17
	Refrigerant - Freon 12	Refrigerant	48.5794	KLB/H	$0.10	USD/Ton-H	$2.43	USD/H	$20,403.35
	Steam @100PSI	Steam	4.60524	KLB/H	$4.14	USD/1000lbs	$19.07	USD/H	$160,151.83
STEP 3	Electricity		80.668	KW	$0.06	USD/KW-H	$4.84	USD/H	$40,656.67
	Cooling Water	Water	292277	GAL/H	$0.08	USD/1000gal	$21.92	USD/H	$184,134.51
	Steam @400PSI	Steam	20.71821	KLB/H	$6.41	USD/1000lbs	$132.80	USD/H	$1,115,551.30
Total Utility Costs (CE Index Adjusted)									**$2,545,165.33**

Total Fixed Costs

Utilities	**Total Utility Costs**	**$2,545,165.33**
Labor-related Operations	Days of Operation	350
	Hours of operation per year	8400
	Hours of operation per week	168
	Operator hours per week	40
	Operators shifts per week	4.2
	due to sickness/vacation, assume:	5
	Number of sections	2
	Operators per section table 23.3	1
	Total operators per shift	2
	Hours per shift	8
	Weeks of operation	50
	Wage	$35.00
	Texas/Gulf cost factor	1
	Direct wages & benefits	$700,000.00
	Direct salaries & benefits	$105,000.00
	Operating supplies and services	$42,000.00
	Technical assistance to manufacturing	$300,000.00
	Control laboratory	$325,000.00
	Total Operations Annual Cost, O	**$1,472,000.00**
Maintenance	Total Depreciable Capital - from TCI page	$65,417,988.11
	Maintenance wage & benefits	$2,747,555.50
	Salaries & benefits	$824,266.65
	Materials & services	$3,297,066.60
	Maintenance overhead	$164,853.33
	Total Annual Maintenance Costs, M	**$7,033,742.08**
Operating Overhead	DW&B	$700,000.00
	Direct salaries and benefits	$105,000.00
	MW&B	$2,747,555.50
	Maintenance salaries and benefits	$824,266.65
	Total Annual M&O-SW&B	**$4,376,822.15**
	General plant overhead	$310,754.37
	Mechanical department services	$105,043.73

	Employee relations department	$258,232.51
	Business services	$323,884.84
	Total Annual Operating Overhead, O	**$997,915.45**
Property Taxes & Insurance	**Total Property Taxes & Insurance**	**$1,308,359.76**
Depreciation	Please see MACRS depreciation in Cash Flow (not in COM)	
	Total Cost of Manufacture, COM	**$13,357,182.62**
	Total Fixed Costs	**$13,357,182.62**

Total Variable Costs and Total Variable Revenues

	Name	**Cost**	**Unit**	**lbs/yr**	**Total Cost**
Raw Materials	Ethylene Oxide	$0.75	USD/lb	203511000	$152,633,250.00
	Carbon Monoxide	$0.10	USD/lb	126545146.6	$12,654,514.66
	MEHQ	$5.00	USD/lb	100800	$504,000.00
				Cost of Raw Materials	**$165,791,764.66**
Product Sales	Acrylic Acid	$1.00	USD/lb	300000000	$300,000,000.00
General Expenses	Selling/Transfer expense	3%			
	Direct Research	4.8%			
	Allocated Research	0.5%			
	Administrative Expenses	2%			
	Management incentive compensation	1.25%			
	Total General Expenses as a function of Revenues	12%			$36,000,000.00
				Total Variable Costs	**$201,791,764.66**
				Total Variable Revenues	**$300,000,000.00**

Cash Flow

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2015	0%	-$120,274,816.16						-$120,274,816.16	$0.00	$0.00	-$120,274,816.16
2016	50%		0.2	-$13,083,597.62	-$13,357,182.62	-$100,895,882.33	$150,000,000.00	$35,746,935.05	$22,663,337.43	-$9,065,334.97	$26,681,600.08
2017	100%		0.32	-$20,933,756.20	-$13,757,898.10	-$207,845,517.60	$309,000,000.00	$87,396,584.30	$66,462,828.11	-$26,585,131.24	$60,811,453.06
2018	100%		0.192	-$12,560,253.72	-$14,170,635.04	-$214,080,883.12	$318,270,000.00	$90,018,481.83	$77,458,228.11	-$30,983,291.25	$59,035,190.59
2019	100%		0.1152	-$7,536,152.23	-$14,595,754.10	-$220,503,309.62	$327,818,100.00	$92,719,036.29	$85,182,884.06	-$34,073,153.62	$58,645,882.66
2020	100%		0.1152	-$7,536,152.23	-$15,033,626.72	-$227,118,408.91	$337,652,643.00	$95,500,607.38	$87,964,455.14	-$35,185,782.06	$60,314,825.32
2021	100%		0.0576	-$3,768,076.12	-$15,484,635.52	-$233,931,961.17	$347,782,222.29	$98,365,625.60	$94,597,549.48	-$37,839,019.79	$60,526,605.80
2022	100%				-$15,949,174.59	-$240,949,920.01	$358,215,688.96	$101,316,594.36	$101,316,594.36	-$40,526,637.75	$60,789,956.62
2023	100%				-$16,427,649.82	-$248,178,417.61	$368,962,159.63	$104,356,092.20	$104,356,092.20	-$41,742,436.88	$62,613,655.32
2024	100%				-$16,920,479.32	-$255,623,770.14	$380,031,024.42	$107,486,774.96	$107,486,774.96	-$42,994,709.98	$64,492,064.98
2025	100%				-$17,428,093.70	-$263,292,483.24	$391,431,955.15	$110,711,378.21	$110,711,378.21	-$44,284,551.28	$66,426,826.93
2026	100%				-$17,950,936.51	-$271,191,257.74	$403,174,913.80	$114,032,719.56	$114,032,719.56	-$45,613,087.82	$68,419,631.73
2027	100%				-$18,489,464.60	-$279,326,995.47	$415,270,161.22	$117,453,701.14	$117,453,701.14	-$46,981,480.46	$70,472,220.69
2028	100%				-$19,044,148.54	-$287,706,805.33	$427,728,266.05	$120,977,312.18	$120,977,312.18	-$48,390,924.87	$72,586,387.31
2029	100%				-$19,615,473.00	-$296,338,009.49	$440,560,114.04	$124,606,631.54	$124,606,631.54	-$49,842,652.62	$74,763,978.93
2030	100%				-$20,203,937.19	-$305,228,149.78	$453,776,917.46	$128,344,830.49	$128,344,830.49	-$51,337,932.20	$77,006,898.29
2031	100%				-$20,810,055.30	-$314,384,994.27	$467,390,224.98	$132,195,175.40	$132,195,175.40	-$52,878,070.16	$79,317,105.24
2032	100%				-$21,434,356.96	-$323,816,544.10	$481,411,931.73	$136,161,030.67	$136,161,030.67	-$54,464,412.27	$81,696,618.40
2033	100%				-$22,077,387.67	-$333,531,040.42	$495,854,289.68	$140,245,861.59	$140,245,861.59	-$56,098,344.63	$84,147,516.95
2034	100%				-$22,739,709.30	-$343,536,971.64	$510,729,918.37	$144,453,237.43	$144,453,237.43	-$57,781,294.97	$86,671,942.46
2035	100%				-$23,421,900.58	-$353,843,080.79	$526,051,815.92	$148,786,834.56	$148,786,834.56	-$59,514,733.82	$89,272,100.73
2036	100%				-$24,124,557.60	-$364,458,373.21	$541,833,370.40	$153,250,439.59	$153,250,439.59	-$61,300,175.84	$91,950,263.76
2037	100%				-$24,848,294.33	-$375,392,124.41	$558,088,371.51	$157,847,952.78	$157,847,952.78	-$63,139,181.11	$94,708,771.67
2038	100%				-$25,593,743.16	-$386,653,888.14	$574,831,022.66	$162,583,391.36	$162,583,391.36	-$65,033,356.55	$97,550,034.82
2039	100%				-$26,361,555.45	-$398,253,504.78	$592,075,953.34	$167,460,893.11	$167,460,893.11	-$66,984,357.24	$100,476,535.86
2040	100%				-$27,152,402.11	-$410,201,109.92	$609,838,231.94	$172,484,719.90	$172,484,719.90	-$68,993,887.96	$103,490,831.94

Year	Plant Capacity	Total Capital Investment	MACRS depreciation	Depreciation Costs	Total Fixed Costs	Total Variable Costs	Acrylic Acid Revenues	BTCF	Taxable Income	Taxes (40%)	ATCF
2041	100%				-$27,966,974.18	-$422,507,143.22	$628,133,378.90	$177,659,261.50	$177,659,261.50	-$71,063,704.60	$106,595,556.90
2042	100%				-$28,805,983.40	-$435,182,357.52	$646,977,380.26	$182,989,039.34	$182,989,039.34	-$73,195,615.74	$109,793,423.60
2043	100%				-$29,670,162.91	-$448,237,828.24	$666,386,701.67	$188,478,710.52	$188,478,710.52	-$75,391,484.21	$113,087,226.31
2044	100%				-$30,560,267.79	-$461,684,963.09	$686,378,302.72	$194,133,071.84	$194,133,071.84	-$77,653,228.73	$116,479,843.10
2045	100%				-$31,477,075.83	-$475,535,511.99	$706,969,651.80	$199,957,063.99	$199,957,063.99	-$79,982,825.60	$119,974,238.39
2046	100%				-$32,421,388.10	-$489,801,577.34	$728,178,741.36	$205,955,775.91	$205,955,775.91	-$82,382,310.36	$123,573,465.55
2047	100%				-$33,394,029.74	-$504,495,624.66	$750,024,103.60	$212,134,449.19	$212,134,449.19	-$84,853,779.68	$127,280,669.51
2048	100%				-$34,395,850.64	-$519,630,493.40	$772,524,826.71	$218,498,482.66	$218,498,482.66	-$87,399,393.07	$131,099,089.60
2049	100%				-$35,427,726.16	-$535,219,408.21	$795,700,571.51	$225,053,437.14	$225,053,437.14	-$90,021,374.86	$135,032,062.29
2050	100%				-$36,490,557.94	-$551,275,990.45	$819,571,588.65	$231,805,040.26	$231,805,040.26	-$92,722,016.10	$139,083,024.15
										Net Present Value	**$287,456,509.12**
										IRR	**42.17%**

APPENDIX E: ASPEN Reports

Section 100 ASPEN Stream Report

S-101 S-102 S-103 S-104 S-105

STREAM ID	S-101	S-102	S-103	S-104	S-105
FROM :	----	----	M-101	H-101	R-101
TO :	M-101	M-101	H-101	R-101	M-102
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
ETHYLENE	636.8000	0.0	3061.0753	3061.0753	2448.8602
OXYGEN	0.0	458.6950	1088.9149	1088.9149	636.6411
ETHYL-OX	0.0	0.0	2.9604	2.9604	553.9539
FORMADEH	0.0	0.0	149.2790	149.2790	152.3401
ACETALDE	0.0	0.0	7.9679-04	7.9679-04	1.5313
CARBONDI	0.0	0.0	49.1401	49.1401	165.4609
WATER	0.0	0.0	4.6050	4.6050	120.9258
ARGON	0.0	2.3050	228.3799	228.3799	228.3799
METHANE	3.2000	0.0	317.2733	317.2733	317.2733
POTAS-01	0.0	0.0	0.0	0.0	0.0
POTAS-02	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	640.0000	461.0000	4901.6286	4901.6286	4625.3665
LB/HR	1.7916+04	1.4770+04	1.4179+05	1.4179+05	1.4179+05
CUFT/HR	1.4017+04	1.0097+04	1.9954+05	1.6511+05	1.6114+05
STATE VARIABLES:					
TEMP F	152.6000	152.6000	71.4073	482.0000	482.0000
PRES PSIA	300.0000	300.0000	140.0000	300.0000	290.0755
VFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
LFRAC	0.0	0.0	0.0	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	2.3115+04	531.1837	8351.5872	1.2835+04	931.3512

```
   BTU/LB                 825.7102    16.5795   288.7108   443.6835
30.3818
   BTU/HR                1.4793+07  2.4488+05  4.0936+07  6.2910+07
4.3078+06
 ENTROPY:
   BTU/LBMOL-R            -17.3061    -5.0013   -11.5280    -6.8887    -
8.5925
   BTU/LB-R                -0.6182    -0.1561    -0.3985    -0.2381    -
0.2803
 DENSITY:
   LBMOL/CUFT            4.5659-02  4.5659-02  2.4565-02  2.9687-02  2.8705-
02
   LB/CUFT                  1.2782     1.4628     0.7106     0.8588
0.8799
 AVG MW                    27.9937    32.0385    28.9272    28.9272
30.6549

 S-106 S-107 S-108 S-109 S-110
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 STREAM ID                  S-106      S-107      S-108      S-109      S-110
 FROM :                     H-105      M-102      H-102      M-103      D-101
 TO   :                     M-102      H-102      D-101      D-101      D-102


 MAX CONV. ERROR:            0.0        0.0    -6.2332-06  9.9909-05     0.0
 SUBSTREAM: MIXED
 PHASE:                     VAPOR      VAPOR      MIXED      LIQUID
LIQUID
 COMPONENTS: LBMOL/HR
   ETHYLENE              4.0044-02  2448.9003  2448.9003     0.3204
1524.4831
   OXYGEN                1.2434-05   636.6411   636.6450  9.9476-05
44.3017
   ETHYL-OX                 0.2022   554.1561   554.1561     1.6172
555.5543
   FORMADEH                 0.4688   152.8089   152.8086     3.7505
156.2712
   ACETALDE              1.1553-03     1.5325     1.5325  9.2416-03
1.5410
   CARBONDI              1.2710-03   165.4622   165.4622  1.0168-02
105.8388
   WATER                  999.2865  1120.2123  1120.2123  7999.2919
9114.8522
   ARGON                 4.0837-06   228.3799   228.3798  3.2670-05
15.3205
   METHANE               6.1989-05   317.2733   317.2730  4.9592-04
44.8201
   POTAS-01                 0.0        0.0        0.0        0.0        0.0
   POTAS-02                 0.0        0.0        0.0        0.0        0.0
 TOTAL FLOW:
   LBMOL/HR              1000.0000  5625.3665  5625.3698  8005.0000
1.1563+04
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   LB/HR                1.8027+04  1.5982+05  1.5982+05  1.4430+05
2.4361+05
   CUFT/HR              1.6988+04  1.8416+05  1.0962+05  2344.7049
4730.2966
 STATE VARIABLES:
   TEMP   F                1.0000   425.2170    94.0183    91.4636
110.3894
   PRES   PSIA           291.0000   290.0755   215.0000   334.0000
200.9000
   VFRAC                   1.0000     1.0000     0.7000     0.0        0.0
   LFRAC                   0.0        0.0        0.3000     1.0000
1.0000
   SFRAC                   0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL           -1.0453+05 -1.7816+04 -2.5641+04 -1.2256+05 -
9.7482+04
   BTU/LB              -5798.5837  -627.0998  -902.5376 -6799.1036 -
4626.9297
   BTU/HR              -1.0453+08 -1.0022+08 -1.4424+08 -9.8113+08 -
1.1272+09
 ENTROPY:
   BTU/LBMOL-R           -17.7479    -9.1566   -19.8641   -38.4732   -
34.1775
   BTU/LB-R               -0.9845    -0.3223    -0.6992    -2.1342    -
1.6222
 DENSITY:
   LBMOL/CUFT           5.8864-02  3.0547-02  5.1318-02     3.4141
2.4445
   LB/CUFT                 1.0611     0.8678     1.4580    61.5443
51.5009
 AVG MW                   18.0266    28.4100    28.4100    18.0266
21.0685

 S-111 S-112 S-113 S-114 S-115
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 STREAM ID                S-111      S-112      S-113      S-114      S-115
 FROM :                   D-101      D-102      D-102      H-103      D-103
 TO   :                   SP-101     M-104      H-103      D-103      D-104

 SUBSTREAM: MIXED
 PHASE:                   VAPOR      LIQUID     VAPOR      MIXED
LIQUID
 COMPONENTS: LBMOL/HR
   ETHYLENE              924.7375     0.3652  1524.1179  1524.1179  6.2453-
19
   OXYGEN                592.3434  1.1341-04    44.3016    44.3016     0.0
   ETHYL-OX                0.2190     1.2923   554.2620   554.2620
551.4907
   FORMADEH                0.2879     4.2520   152.0192   152.0192
1.5202
   ACETALDE             7.5274-04  2.5245-04     1.5407     1.5407
1.5407
```

CARBONDI	59.6336	1.1593-02	105.8272	105.8272	5.0684-21
WATER	4.6519	7994.0779	1120.7743	1120.7743	1120.7743
ARGON	213.0594	3.7247-05	15.3204	15.3204	0.0
METHANE	272.4534	5.6539-04	44.8196	44.8196	2.0667-32
POTAS-01	0.0	0.0	0.0	0.0	0.0
POTAS-02	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	2067.3868	8000.0000	3562.9830	3562.9830	1675.3259
LB/HR	6.0505+04	1.4421+05	9.9404+04	9.9404+04	4.4599+04
CUFT/HR	6.1177+04	2796.9697	1.8845+05	7776.1372	830.9904
STATE VARIABLES:					
TEMP F	91.8244	357.8672	279.6351	-28.6444	191.5496
PRES PSIA	200.0000	150.3000	150.0000	145.0000	142.9000
VFRAC	1.0000	0.0	1.0000	5.0000-02	0.0
LFRAC	0.0	1.0000	0.0	0.9500	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	877.9876	-1.1718+05	-3.2441+04	-4.5842+04	-9.0578+04
BTU/LB	29.9996	-6500.7327	-1162.8119	-1643.1361	-3402.4705
BTU/HR	1.8151+06	-9.3748+08	-1.1559+08	-1.6333+08	-1.5175+08
ENTROPY:					
BTU/LBMOL-R	-10.5474	-30.7918	-12.3415	-34.4043	-38.5537
BTU/LB-R	-0.3604	-1.7082	-0.4424	-1.2332	-1.4482
DENSITY:					
LBMOL/CUFT	3.3793-02	2.8602	1.8906-02	0.4582	2.0161
LB/CUFT	0.9890	51.5597	0.5275	12.7832	53.6703
AVG MW	29.2666	18.0264	27.8990	27.8990	26.6214

S-116 S-117 S-118 S-119 S-120

STREAM ID	S-116	S-117	S-118	S-119	S-120
FROM :	D-103	D-104	D-104	M-104	SP-103
TO :	M-105	M-104	----	SP-103	H-104

SUBSTREAM: MIXED

PHASE:	VAPOR	LIQUID	VAPOR	MIXED	MIXED
COMPONENTS: LBMOL/HR					
ETHYLENE	1524.1179	0.0	0.0	0.3652	0.3204
OXYGEN	44.3016	0.0	0.0	1.1341-04	9.9475-05
ETHYL-OX	2.7713	0.5515	550.9392	1.8438	1.6172
FORMADEH	150.4990	2.3997-02	1.4962	4.2760	3.7505
ACETALDE	5.2171-05	1.0285-02	1.5304	1.0537-02	9.2425-03
CARBONDI	105.8272	0.0	0.0	1.1593-02	1.0168-02
WATER	1.5690-09	1120.2139	0.5604	9114.2918	7994.2919
ARGON	15.3204	0.0	0.0	3.7247-05	3.2670-05
METHANE	44.8196	0.0	0.0	5.6539-04	4.9592-04
POTAS-01	0.0	0.0	0.0	0.0	0.0
POTAS-02	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	1887.6571	1120.7997	554.5262	9120.7997	8000.0000
LB/HR	5.4804+04	2.0206+04	2.4393+04	1.6442+05	1.4421+05
CUFT/HR	6.7031+04	357.0901	1.5615+05	4.2657+05	3.7415+05
STATE VARIABLES:					
TEMP F	3.5867	231.7415	65.1356	233.1496	233.1496
PRES PSIA	140.0000	22.1000	20.0000	22.1000	22.1000
VFRAC	1.0000	0.0	1.0000	0.1382	0.1382
LFRAC	0.0	1.0000	0.0	0.8618	0.8618
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	2502.4196	-1.1993+05	-2.3083+04	-1.1752+05	-1.1752+05
BTU/LB	86.1923	-6652.2639	-524.7555	-6519.3554	-6519.3554
BTU/HR	4.7237+06	-1.3442+08	-1.2800+07	-1.0719+09	-9.4018+08
ENTROPY:					
BTU/LBMOL-R	-14.9339	-34.2830	-32.2109	-30.7924	-30.7924
BTU/LB-R	-0.5144	-1.9016	-0.7322	-1.7082	-1.7082
DENSITY:					
LBMOL/CUFT	2.8161-02	3.1387	3.5512-03	2.1382-02	2.1382-02

LB/CUFT	0.8176	56.5864	0.1562	0.3854	0.3854
AVG MW	29.0330	18.0286	43.9890	18.0266	18.0266

S-121 S-122 S-123 S-124 S-125

STREAM ID	S-121	S-122	S-123	S-124	S-125
FROM :	SP-103	SP-103	H-104	P-101	----
TO :	----	H-105	P-101	M-103	M-103
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
ETHYLENE	4.8373-03	4.0044-02	0.3204	0.3204	0.0
OXYGEN	1.5021-06	1.2434-05	9.9475-05	9.9475-05	0.0
ETHYL-OX	2.4420-02	0.2022	1.6172	1.6172	0.0
FORMADEH	5.6633-02	0.4688	3.7505	3.7505	0.0
ACETALDE	1.3956-04	1.1553-03	9.2425-03	9.2425-03	0.0
CARBONDI	1.5354-04	1.2710-03	1.0168-02	1.0168-02	0.0
WATER	120.7135	999.2865	7994.2919	7994.2919	5.0000
ARGON	4.9331-07	4.0837-06	3.2670-05	3.2670-05	0.0
METHANE	7.4883-06	6.1989-05	4.9592-04	4.9592-04	0.0
POTAS-01	0.0	0.0	0.0	0.0	0.0
POTAS-02	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	120.7997	1000.0000	8000.0000	8000.0000	5.0000
LB/HR	2177.6127	1.8027+04	1.4421+05	1.4421+05	90.0764
CUFT/HR	5649.6417	4.6769+04	2341.3624	2343.2428	1.4619
STATE VARIABLES:					
TEMP F	233.1496	233.1496	90.0000	91.4643	90.0000
PRES PSIA	22.1000	22.1000	15.0000	334.0000	334.0000
VFRAC	0.1382	0.1382	0.0	0.0	0.0
LFRAC	0.8618	0.8618	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.1752+05	-1.1752+05	-1.2259+05	-1.2256+05	-1.2264+05
BTU/LB	-6519.3554	-6519.3554	-6800.5490	-6799.0983	-6807.5962
BTU/HR	-1.4197+07	-1.1752+08	-9.8073+08	-9.8052+08	-6.1320+05
ENTROPY:					
BTU/LBMOL-R	-30.7924	-30.7924	-38.5205	-38.4732	-38.5412

BTU/LB-R	-1.7082	-1.7082	-2.1369	-2.1342	-2.1394
DENSITY:					
LBMOL/CUFT	2.1382-02	2.1382-02	3.4168	3.4141	3.4201
LB/CUFT	0.3854	0.3854	61.5937	61.5442	61.6141
AVG MW	18.0266	18.0266	18.0266	18.0266	18.0153

S-126 S-127 S-128 S-129 S-130

STREAM ID	S-126	S-127	S-128	S-129	S-130
FROM :	SP-101	SP-101	M-105	SP-102	SP-102
TO :	----	M-105	SP-102	----	CO2SCRUB
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	MIXED	MIXED	MIXED
COMPONENTS: LBMOL/HR					
ETHYLENE	9.2474-02	924.6450	2448.7629	24.4876	2424.2753
OXYGEN	5.9234-02	592.2842	636.5858	6.3659	630.2199
ETHYL-OX	2.1898-05	0.2190	2.9903	2.9903-02	2.9604
FORMADEH	2.8791-05	0.2879	150.7869	1.5079	149.2790
ACETALDE	7.5274-08	7.5266-04	8.0483-04	8.0483-06	7.9679-04
CARBONDI	5.9634-03	59.6276	165.4548	1.6545	163.8003
WATER	4.6519-04	4.6515	4.6515	4.6515-02	4.6050
ARGON	2.1306-02	213.0381	228.3585	2.2836	226.0749
METHANE	2.7245-02	272.4261	317.2457	3.1725	314.0733
POTAS-01	0.0	0.0	0.0	0.0	0.0
POTAS-02	0.0	0.0	0.0	0.0	0.0
TOTAL FLOW:					
LBMOL/HR	0.2067	2067.1801	3954.8372	39.5484	3915.2888
LB/HR	6.0505	6.0499+04	1.1530+05	1153.0372	1.1415+05
CUFT/HR	6.1177	6.1171+04	1.5392+05	1539.1778	1.5238+05
STATE VARIABLES:					
TEMP F	91.8244	91.8244	48.2559	48.2559	48.2559
PRES PSIA	200.0000	200.0000	140.0000	140.0000	140.0000

```
   VFRAC                     1.0000     1.0000     0.9996     0.9996
0.9996
   LFRAC                     0.0        0.0      3.9246-04  3.9246-04  3.9246-
04
   SFRAC                     0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL               877.9876   877.9876  1653.3345  1653.3345
1653.3345
   BTU/LB                   29.9996    29.9996    56.7082    56.7082
56.7082
   BTU/HR                  181.5140  1.8150+06  6.5387+06  6.5387+04
6.4733+06
 ENTROPY:
   BTU/LBMOL-R             -10.5474   -10.5474   -11.9074   -11.9074   -
11.9074
   BTU/LB-R                 -0.3604    -0.3604    -0.4084    -0.4084    -
0.4084
 DENSITY:
   LBMOL/CUFT             3.3793-02  3.3793-02  2.5694-02  2.5694-02  2.5694-
02
   LB/CUFT                   0.9890     0.9890     0.7491     0.7491
0.7491
 AVG MW                     29.2666    29.2666    29.1551    29.1551
29.1551

 S-131 S-132
 -----------

 STREAM ID                  S-131      S-132
 FROM :                     CO2SCRUB   CO2SCRUB
 TO   :                     ----       M-101

 SUBSTREAM: MIXED
 PHASE:                     VAPOR      MIXED
 COMPONENTS: LBMOL/HR
   ETHYLENE                  0.0      2424.2753
   OXYGEN                    0.0       630.2199
   ETHYL-OX                  0.0         2.9604
   FORMADEH                  0.0       149.2790
   ACETALDE                  0.0      7.9679-04
   CARBONDI                114.6602     49.1401
   WATER                     0.0         4.6050
   ARGON                     0.0       226.0749
   METHANE                   0.0       314.0733
   POTAS-01                  0.0         0.0
   POTAS-02                  0.0         0.0
 TOTAL FLOW:
   LBMOL/HR                114.6602  3800.6286
   LB/HR                  5046.1723  1.0910+05
   CUFT/HR                4464.1789  1.4791+05
 STATE VARIABLES:
   TEMP   F                 48.2559    48.2559
   PRES   PSIA             140.0000   140.0000
   VFRAC                     1.0000     0.9996
```

LFRAC	0.0	4.4282-04
SFRAC	0.0	0.0
ENTHALPY:		
BTU/LBMOL	-1.6943+05	6814.1631
BTU/LB	-3849.8622	237.3697
BTU/HR	-1.9427+07	2.5898+07
ENTROPY:		
BTU/LBMOL-R	-4.2714	-12.3571
BTU/LB-R	-9.7056-02	-0.4305
DENSITY:		
LBMOL/CUFT	2.5684-02	2.5696-02
LB/CUFT	1.1304	0.7376
AVG MW	44.0098	28.7070

Section 200 ASPEN Stream Report

S-201 S-202 S-203 S-204 S-205

STREAM ID	S-201	S-202	S-203	S-204	S-205
FROM :	----	----	----	----	----
TO :	R-201	R-201	R-201	R-202	R-202
SUBSTREAM: MIXED					
PHASE:	MIXED	LIQUID	LIQUID	MIXED	LIQUID
COMPONENTS: LBMOL/HR					
CO	235.8447	0.5300	0.0	235.8447	0.5300
BETA--01	0.0	0.0	0.0	0.0	0.0
ETHYL-01	179.2796	17.6670	0.0	179.2796	17.6670
SULFO-01	0.0	0.0	1879.7692	0.0	0.0
ACETA-01	1.7928	3.2000	0.0	1.7928	3.2000
TOTAL FLOW:					
LBMOL/HR	416.9171	21.3970	1879.7692	416.9171	21.3970
LB/HR	1.4583+04	934.1028	2.2590+05	1.4583+04	934.1028
CUFT/HR	3345.4096	19.9726	2970.2314	3345.4096	19.9726
STATE VARIABLES:					
TEMP C	80.0000	80.0000	80.0000	80.0000	80.0000
PRES PSIA	614.6959	614.6959	614.6959	614.6959	614.6959
VFRAC	0.6982	0.0	0.0	0.6982	0.0
LFRAC	0.3018	1.0000	1.0000	0.3018	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-3.8739+04	-3.8657+04	-1.8579+05	-3.8739+04	-3.8657+04
BTU/LB	-1107.5374	-885.4980	-1546.0128	-1107.5374	-885.4980
BTU/HR	-1.6151+07	-8.2715+05	-3.4924+08	-1.6151+07	-8.2715+05
ENTROPY:					
BTU/LBMOL-R	-10.0788	-44.9867	-128.2942	-10.0788	-44.9867
BTU/LB-R	-0.2881	-1.0305	-1.0676	-0.2881	-1.0305
DENSITY:					
LBMOL/CUFT	0.1246	1.0713	0.6329	0.1246	1.0713

LB/CUFT	4.3591	46.7691	76.0534	4.3591	46.7691
AVG MW	34.9780	43.6558	120.1723	34.9780	43.6558

S-206 S-207 S-208 S-209 S-210

STREAM ID	S-206	S-207	S-208	S-209	S-210
FROM :	----	----	----	----	R-201
TO :	R-202	R-203	R-203	R-203	M-201
SUBSTREAM: MIXED					
PHASE:	LIQUID	MIXED	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
CO	0.0	235.8447	0.5300	0.0	63.2016
BETA--01	0.0	0.0	0.0	0.0	173.1731
ETHYL-01	0.0	179.2796	17.6670	0.0	18.7015
SULFO-01	1879.7692	0.0	0.0	1879.7692	1879.7692
ACETA-01	0.0	1.7928	3.2000	0.0	10.0648
TOTAL FLOW:					
LBMOL/HR	1879.7692	416.9171	21.3970	1879.7692	2144.9102
LB/HR	2.2590+05	1.4583+04	934.1028	2.2590+05	2.4141+05
CUFT/HR	2970.2314	3345.4096	19.9726	2970.2314	3256.5620
STATE VARIABLES:					
TEMP C	80.0000	80.0000	80.0000	80.0000	80.0000
PRES PSIA	614.6959	614.6959	614.6959	614.6959	614.6959
VFRAC	0.0	0.6982	0.0	0.0	0.0
LFRAC	1.0000	0.3018	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.8579+05	-3.8739+04	-3.8657+04	-1.8579+05	-1.7606+05
BTU/LB	-1546.0128	-1107.5374	-885.4980	-1546.0128	-1564.2952
BTU/HR	-3.4924+08	-1.6151+07	-8.2715+05	-3.4924+08	-3.7764+08
ENTROPY:					
BTU/LBMOL-R	-128.2942	-10.0788	-44.9867	-128.2942	-117.3603
BTU/LB-R	-1.0676	-0.2881	-1.0305	-1.0676	-1.0427

DENSITY:					
LBMOL/CUFT	0.6329	0.1246	1.0713	0.6329	0.6586
LB/CUFT	76.0534	4.3591	46.7691	76.0534	74.1313
AVG MW	120.1723	34.9780	43.6558	120.1723	112.5517

S-211 S-212 S-213 S-214 S-215

STREAM ID	S-211	S-212	S-213	S-214	S-215
FROM :	R-202	R-203	M-201	D-201	D-201
TO :	M-201	M-201	D-201	K-201	D-202
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID
COMPONENTS: LBMOL/HR					
CO	63.2016	63.2016	189.6049	189.6049	8.7686-24
BETA--01	173.1731	173.1731	519.5192	1.0158-02	519.5091
ETHYL-01	18.7015	18.7015	56.1045	56.1045	8.1322-10
SULFO-01	1879.7692	1879.7692	5639.3075	1.0917-34	5639.3075
ACETA-01	10.0648	10.0648	30.1944	30.1944	3.0577-09
TOTAL FLOW:					
LBMOL/HR	2144.9102	2144.9102	6434.7306	275.9140	6158.8166
LB/HR	2.4141+05	2.4141+05	7.2424+05	9113.3815	7.1513+05
CUFT/HR	3256.5620	3256.5620	9769.6858	3.5770+05	1.0730+04
STATE VARIABLES:					
TEMP C	80.0000	80.0000	80.0000	-24.8280	232.0580
PRES PSIA	614.6959	614.6959	614.6959	3.7000	6.8500
VFRAC	0.0	0.0	0.0	1.0000	0.0
LFRAC	1.0000	1.0000	1.0000	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.7606+05	-1.7606+05	-1.7606+05	-4.6051+04	-1.6772+05
BTU/LB	-1564.2952	-1564.2952	-1564.2952	-1394.2349	-1444.4615
BTU/HR	-3.7764+08	-3.7764+08	-1.1329+09	-1.2706+07	-1.0330+09
ENTROPY:					

BTU/LBMOL-R	-117.3603	-117.3603	-117.3603	8.1802	-104.4561
BTU/LB-R	-1.0427	-1.0427	-1.0427	0.2477	-0.8996
DENSITY:					
LBMOL/CUFT	0.6586	0.6586	0.6586	7.7136-04	0.5740
LB/CUFT	74.1313	74.1313	74.1313	2.5478-02	66.6502
AVG MW	112.5517	112.5517	112.5517	33.0298	116.1142

S-216 S-217 S-218 S-219 S-220

STREAM ID	S-216	S-217	S-218	S-219	S-220
FROM :	D-202	H-201	H-202	D-202	H-203
TO :	H-201	H-202	----	H-203	H-204
SUBSTREAM: MIXED					
PHASE:	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
CO	0.0	0.0	0.0	0.0	0.0
BETA--01	518.5248	518.5248	518.5248	0.9843	0.9843
ETHYL-01	8.1322-10	8.1322-10	8.1322-10	2.3460-23	2.3460-23
SULFO-01	0.9892	0.9892	0.9892	5638.3183	5638.3183
ACETA-01	3.0577-09	3.0577-09	3.0577-09	3.9598-22	3.9598-22
TOTAL FLOW:					
LBMOL/HR	519.5140	519.5140	519.5140	5639.3026	5639.3026
LB/HR	3.7486+04	3.7486+04	3.7486+04	6.7764+05	6.7764+05
CUFT/HR	1.9401+06	564.3733	531.6218	1.0137+04	1.0132+04
STATE VARIABLES:					
TEMP C	113.5126	100.7470	37.7778	240.8118	240.2902
PRES PSIA	2.0000	2.0000	2.0000	3.5000	614.6959
VFRAC	1.0000	0.0	0.0	0.0	0.0
LFRAC	0.0	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-1.1865+05	-1.3777+05	-1.4128+05	-1.7041+05	-1.7046+05
BTU/LB	-1644.4093	-1909.3393	-1958.0465	-1418.1073	-1418.5612

BTU/HR	-6.1642+07	-7.1573+07	-7.3399+07	-9.6097+08	-9.6127+08
ENTROPY:					
BTU/LBMOL-R	-38.2778	-66.6563	-72.1015	-108.5806	-108.6391
BTU/LB-R	-0.5305	-0.9238	-0.9993	-0.9036	-0.9041
DENSITY:					
LBMOL/CUFT	2.6777-04	0.9205	0.9772	0.5563	0.5566
LB/CUFT	1.9321-02	66.4199	70.5118	66.8488	66.8811
AVG MW	72.1552	72.1552	72.1552	120.1639	120.1639

S-221 S-222 S-223 S-224 S-225

STREAM ID	S-221	S-222	S-223	S-224	S-225
FROM :	H-204	SP-203	SP-203	----	SP-202
TO :	SP-203	----	SP-202	SP-202	----
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
CO	0.0	0.0	0.0	0.0	0.0
BETA--01	0.9843	9.8427-04	0.9833	0.0	0.3278
ETHYL-01	2.3460-23	2.3460-26	2.3436-23	0.0	7.8120-24
SULFO-01	5638.3183	5.6383	5632.6800	5.6383	1879.4394
ACETA-01	3.9598-22	3.9598-25	3.9558-22	0.0	1.3186-22
TOTAL FLOW:					
LBMOL/HR	5639.3026	5.6393	5633.6633	5.6383	1879.7672
LB/HR	6.7764+05	677.6407	6.7696+05	677.5700	2.2588+05
CUFT/HR	8910.2207	8.9102	8901.3105	8.9091	2970.0732
STATE VARIABLES:					
TEMP C	80.0000	80.0000	80.0000	80.0000	80.0000
PRES PSIA	614.6959	614.6959	614.6959	614.6959	614.6959
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:					

BTU/LBMOL	-1.8578+05	-1.8578+05	-1.8578+05	-1.8579+05	-1.8578+05
BTU/LB	-1546.0527	-1546.0527	-1546.0527	-1546.0128	-1546.0527
BTU/HR	-1.0477+09	-1.0477+06	-1.0466+09	-1.0475+06	-3.4922+08
ENTROPY:					
BTU/LBMOL-R	-128.2804	-128.2804	-128.2804	-128.2942	-128.2804
BTU/LB-R	-1.0675	-1.0675	-1.0675	-1.0676	-1.0675
DENSITY:					
LBMOL/CUFT	0.6329	0.6329	0.6329	0.6329	0.6329
LB/CUFT	76.0521	76.0521	76.0521	76.0534	76.0521
AVG MW	120.1639	120.1639	120.1639	120.1723	120.1639

S-226 S-227 S-228 S-229 S-230

STREAM ID	S-226	S-227	S-228	S-229	S-230
FROM :	SP-202	SP-202	K-201	D-203	F-201
TO :	----	----	D-203	F-201	H-203
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	VAPOR	LIQUID
COMPONENTS: LBMOL/HR					
CO	0.0	0.0	189.6049	189.6049	5.0171
BETA--01	0.3278	0.3278	1.0158-02	1.0229-28	0.0
ETHYL-01	7.8120-24	7.8120-24	56.1045	54.5900	53.7053
SULFO-01	1879.4394	1879.4394	1.0917-34	0.0	0.0
ACETA-01	1.3186-22	1.3186-22	30.1944	9.8050	9.7147
TOTAL FLOW:					
LBMOL/HR	1879.7672	1879.7672	275.9140	254.0000	68.4372
LB/HR	2.2588+05	2.2588+05	9113.3815	8147.7160	2934.3860
CUFT/HR	2970.0732	2970.0732	5.8311+04	8.7602+04	53.1889
STATE VARIABLES:					
TEMP C	80.0000	80.0000	-30.4200	-10.6874	-20.0000
PRES PSIA	614.6959	614.6959	17.0000	14.7000	614.6959
VFRAC	0.0	0.0	0.7656	1.0000	0.0
LFRAC	1.0000	1.0000	0.2344	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0

ENTHALPY:					
BTU/LBMOL	-1.8578+05	-1.8578+05	-4.8971+04	-4.3688+04	-4.3440+04
BTU/LB	-1546.0527	-1546.0527	-1482.6314	-1361.9365	-1013.1201
BTU/HR	-3.4922+08	-3.4922+08	-1.3512+07	-1.1097+07	-2.9729+06
ENTROPY:					
BTU/LBMOL-R	-128.2804	-128.2804	-1.1886	8.4259	-49.5761
BTU/LB-R	-1.0675	-1.0675	-3.5987-02	0.2627	-1.1562
DENSITY:					
LBMOL/CUFT	0.6329	0.6329	4.7318-03	2.8995-03	1.2867
LB/CUFT	76.0521	76.0521	0.1563	9.3009-02	55.1692
AVG MW	120.1639	120.1639	33.0298	32.0776	42.8771

S-231 S-232 S-233 S-234 S-235

STREAM ID	S-231	S-232	S-233	S-234	S-235
FROM :	H-203	F-202	SP-201	SP-201	SP-201
TO :	F-202	SP-201	----	----	----
SUBSTREAM: MIXED					
PHASE:	MIXED	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
CO	5.0171	1.5938	0.5313	0.5313	0.5313
BETA--01	0.0	0.0	0.0	0.0	0.0
ETHYL-01	53.7053	52.9852	17.6617	17.6617	17.6617
SULFO-01	0.0	0.0	0.0	0.0	0.0
ACETA-01	9.7147	9.6210	3.2070	3.2070	3.2070
TOTAL FLOW:					
LBMOL/HR	68.4372	64.2000	21.4000	21.4000	21.4000
LB/HR	2934.3860	2802.6452	934.2151	934.2151	934.2151
CUFT/HR	106.9523	59.9302	19.9767	19.9767	19.9767
STATE VARIABLES:					
TEMP C	80.0000	80.0000	80.0000	80.0000	80.0000
PRES PSIA	614.6959	614.6959	614.6959	614.6959	614.6959
VFRAC	6.1913-02	0.0	0.0	0.0	0.0

```
   LFRAC                  0.9381     1.0000     1.0000     1.0000
1.0000
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL          -3.8946+04 -3.8673+04 -3.8673+04 -3.8673+04 -
3.8673+04
   BTU/LB              -908.3071  -885.8913  -885.8913  -885.8913  -
885.8913
   BTU/HR             -2.6653+06 -2.4828+06 -8.2761+05 -8.2761+05 -
8.2761+05
 ENTROPY:
   BTU/LBMOL-R          -41.8034   -44.9802   -44.9802   -44.9802   -
44.9802
   BTU/LB-R              -0.9750    -1.0304    -1.0304    -1.0304    -
1.0304
 DENSITY:
   LBMOL/CUFT             0.6399     1.0712     1.0712     1.0712
1.0712
   LB/CUFT               27.4364    46.7652    46.7652    46.7652
46.7652
 AVG MW                  42.8771    43.6549    43.6549    43.6549
43.6549

 S-236 S-237 S-238
 -----------------

 STREAM ID               S-236      S-237      S-238
 FROM :                  D-203      F-201      F-202
 TO   :                  ----       ----       ----

 SUBSTREAM: MIXED
 PHASE:                  LIQUID     VAPOR      VAPOR
 COMPONENTS: LBMOL/HR
   CO                 1.7930-24   184.5878     3.4233
   BETA--01           1.0158-02     0.0        0.0
   ETHYL-01             1.5144      0.8847     0.7201
   SULFO-01             0.0         0.0        0.0
   ACETA-01            20.3894   9.0289-02  9.3719-02
 TOTAL FLOW:
   LBMOL/HR            21.9140    185.5628     4.2372
   LB/HR              965.6655   5213.3300   131.7408
   CUFT/HR             20.1342   1476.1743    47.0221
 STATE VARIABLES:
   TEMP   C            33.8294    -20.0000    80.0000
   PRES   PSIA         16.9500    614.6959   614.6959
   VFRAC                0.0         1.0000     1.0000
   LFRAC                1.0000      0.0        0.0
   SFRAC                0.0         0.0        0.0
 ENTHALPY:
   BTU/LBMOL         -8.0556+04 -4.7978+04 -4.3068+04
   BTU/LB            -1828.0698 -1707.7400 -1385.1806
   BTU/HR            -1.7653+06 -8.9030+06 -1.8248+05
 ENTROPY:
   BTU/LBMOL-R         -46.4795    12.5623     6.3303
```

BTU/LB-R	-1.0548	0.4471	0.2036
DENSITY:			
LBMOL/CUFT	1.0884	0.1257	9.0110-02
LB/CUFT	47.9615	3.5316	2.8017
AVG MW	44.0661	28.0947	31.0918

Section 300 ASPEN Stream Results

S-301 S-302 S-303 S-304 S-305

STREAM ID	S-301	S-302	S-303	S-304	S-305
FROM :	----	----	R-301	----	F-301
TO :	R-301	R-301	F-301	M-301	M-301
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	LIQUID	VAPOR
COMPONENTS: LBMOL/HR					
NITROGEN	0.0	0.0	0.0	0.0	0.0
BETA--01	0.1582	517.7790	15.9406	0.0	15.7823
ORTHO-01	48.0351	0.0	48.0351	0.0	0.0
WATER	0.0	0.0	1.4397-09	0.9000	1.4375-09
ACRYL-01	2.8067	0.0	523.4266	0.0	520.5904
P-MET-01	0.0	0.0	0.8946	0.1000	0.7945
TOTAL FLOW:					
LBMOL/HR	51.0000	517.7790	588.2969	1.0000	537.1672
LB/HR	4920.8701	3.7313+04	4.3687+04	28.6277	3.8752+04
CUFT/HR	112.1776	529.2959	2.3838+06	0.4490	2.3837+06
STATE VARIABLES:					
TEMP F	338.0000	100.0000	338.0000	194.0000	338.0000
PRES PSIA	1.9334	1.9290	1.9290	15.0000	1.9290
VFRAC	0.0	0.0	0.9131	0.0	1.0000
LFRAC	1.0000	1.0000	8.6911-02	1.0000	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-5.1202+05	-1.4119+05	-1.7090+05	-1.2180+05	-1.3852+05
BTU/LB	-5306.5643	-1959.2606	-2301.3281	-4254.5912	-1920.1400
BTU/HR	-2.6113+07	-7.3106+07	-1.0054+08	-1.2180+05	-7.4408+07
ENTROPY:					
BTU/LBMOL-R	247.8420	-72.0103	-3.7957	-44.1400	-27.6661
BTU/LB-R	2.5686	-0.9993	-5.1114-02	-1.5419	-0.3835
DENSITY:					
LBMOL/CUFT	0.4546	0.9782	2.4679-04	2.2271	2.2535-04

```
   LB/CUFT                  43.8668    70.4955  1.8326-02    63.7573  1.6257-
02
  AVG MW                    96.4876    72.0636    74.2601    28.6277
72.1406

  S-306 S-307 S-308 S-309 S-310
  -----------------------------

  STREAM ID                 S-306      S-307      S-308      S-309      S-310
  FROM :                    F-301      M-301      ----       HEATX1
HEATX1
  TO   :                    ----       HEATX1     HEATX1     ----       B1

  SUBSTREAM: MIXED
  PHASE:                    LIQUID     VAPOR      LIQUID     LIQUID
LIQUID
  COMPONENTS: LBMOL/HR
    NITROGEN                 0.0        0.0        0.0        0.0        0.0
    BETA--01                 0.1584    15.7823     0.0        0.0
15.7823
    ORTHO-01                48.0351     0.0        0.0        0.0        0.0
    WATER                2.2653-12     0.9000  6661.0122  6661.0122
0.9000
    ACRYL-01                 2.8362   520.5904     0.0        0.0
520.5904
    P-MET-01                 0.1001     0.8945     0.0        0.0
0.8945
  TOTAL FLOW:
    LBMOL/HR                51.1297   538.1672  6661.0122  6661.0122
538.1672
    LB/HR                 4935.4280  3.8780+04  1.2000+05  1.2000+05
3.8780+04
    CUFT/HR                112.4043  2.3835+06  1947.6067  2028.2409
629.3170
  STATE VARIABLES:
    TEMP   F               338.0000   336.4525    90.0000   160.9913
175.0000
    PRES   PSIA              1.9290     1.9290    73.4797    73.4797
1.9290
    VFRAC                    0.0        1.0000     0.0        0.0        0.0
    LFRAC                    1.0000     0.0        1.0000     1.0000
1.0000
    SFRAC                    0.0        0.0        0.0        0.0        0.0
  ENTHALPY:
    BTU/LBMOL            -5.1105+05 -1.3849+05 -1.2264+05 -1.2135+05 -
1.5452+05
    BTU/LB               -5294.3068 -1921.8633 -6807.5962 -6735.6873 -
2144.3755
    BTU/HR               -2.6130+07 -7.4530+07 -8.1691+08 -8.0828+08 -
8.3159+07
  ENTROPY:
    BTU/LBMOL-R            246.9856   -27.6571   -38.5412   -36.3378   -
51.7161
```

```
   BTU/LB-R                 2.5587    -0.3838    -2.1394    -2.0171    -
0.7177
 DENSITY:
   LBMOL/CUFT               0.4549  2.2579-04     3.4201     3.2841
0.8552
   LB/CUFT                 43.9078  1.6270-02    61.6141    59.1646
61.6227
 AVG MW                    96.5276    72.0597    18.0153    18.0153
72.0597

 S-311 S-312 S-313 S-314 S-315
 -----------------------------

 STREAM ID                 S-311      S-312      S-313      S-314      S-315
 FROM :                    B1         B1         P-301      D-301      D-301
 TO   :                    ----       P-301      D-301      H-302      R-301


 MAX CONV. ERROR:           0.0        0.0    -6.1795-05     0.0        0.0
 SUBSTREAM: MIXED
 PHASE:                    MISSING    LIQUID     LIQUID     VAPOR
LIQUID
 COMPONENTS: LBMOL/HR
   NITROGEN                 0.0        0.0        0.0        0.0        0.0
   BETA--01                 0.0       15.7823    15.7823     2.3649
13.4174
   ORTHO-01                 0.0        0.0        0.0        0.0        0.0
   WATER                    0.0        0.9000     0.9000     0.9000  1.4397-
09
   ACRYL-01                 0.0      520.5904   520.5904   515.3845
5.2059
   P-MET-01                 0.0        0.8945     0.8945  6.9158-09
0.8946
 TOTAL FLOW:
   LBMOL/HR                 0.0      538.1672   538.1672   518.6494
19.5178
   LB/HR                    0.0     3.8780+04  3.8780+04  3.7327+04
1453.1108
   CUFT/HR                  0.0      629.3169   629.6650  1.1806+05
25.1362
 STATE VARIABLES:
   TEMP   F                MISSING   174.9999   175.8338   346.3411
386.6608
   PRES   PSIA              1.8323     1.8323    40.7500    38.0000
42.1000
   VFRAC                   MISSING     0.0        0.0        1.0000     0.0
   LFRAC                   MISSING     1.0000     1.0000     0.0
1.0000
   SFRAC                   MISSING     0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL               MISSING -1.5452+05 -1.5451+05 -1.3888+05 -
1.3574+05
   BTU/LB                  MISSING -2144.3756 -2144.1434 -1929.7269 -
1823.2684
```

BTU/HR	MISSING	-8.3159+07	-8.3150+07	-7.2031+07	-2.6494+06
ENTROPY:					
BTU/LBMOL-R	MISSING	-51.7161	-51.7049	-33.2176	-56.5947
BTU/LB-R	MISSING	-0.7177	-0.7175	-0.4615	-0.7602
DENSITY:					
LBMOL/CUFT	MISSING	0.8552	0.8547	4.3933-03	0.7765
LB/CUFT	MISSING	61.6227	61.5886	0.3162	57.8094
AVG MW	MISSING	72.0597	72.0597	71.9698	74.4504

S-316 S-317 S-318 S-319 S-320

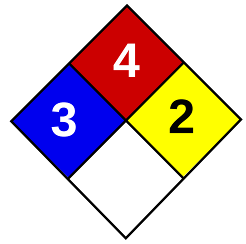
STREAM ID	S-316	S-317	S-318	S-319	S-320
FROM :	----	H-302	----	----	H-302
TO :	H-302	----	F-302	F-302	F-302
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
NITROGEN	0.0	0.0	0.1785	0.0	0.0
BETA--01	0.0	0.0	0.0	0.0	2.3649
ORTHO-01	0.0	0.0	0.0	0.0	0.0
WATER	7000.0000	7000.0000	0.0	0.9000	0.9000
ACRYL-01	0.0	0.0	0.0	0.0	515.3845
P-MET-01	0.0	0.0	0.0	0.1000	6.9158-09
TOTAL FLOW:					
LBMOL/HR	7000.0000	7000.0000	0.1785	1.0000	518.6494
LB/HR	1.2611+05	1.2611+05	5.0000	28.6277	3.7327+04
CUFT/HR	2046.7230	2131.5534	61.9317	0.4206	579.3943
STATE VARIABLES:					
TEMP F	90.0000	161.0640	90.0000	80.0000	100.0000
PRES PSIA	73.4797	73.4797	17.0000	20.0000	17.0000
VFRAC	0.0	0.0	1.0000	0.0	0.0
LFRAC	1.0000	1.0000	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					

```
   BTU/LBMOL          -1.2264+05 -1.2134+05    90.4420 -1.2431+05 -
1.5638+05
   BTU/LB             -6807.5962 -6735.6118     3.2285 -4342.3974 -
2172.9214
   BTU/HR             -8.5849+08 -8.4941+08    16.1426 -1.2431+05 -
8.1109+07
 ENTROPY:
   BTU/LBMOL-R          -38.5412   -36.3356    -0.1227   -48.2208   -
52.1426
   BTU/LB-R              -2.1394    -2.0169 -4.3802-03    -1.6844    -
0.7245
 DENSITY:
   LBMOL/CUFT             3.4201     3.2840  2.8820-03     2.3774
0.8952
   LB/CUFT               61.6141    59.1620  8.0734-02    68.0585
64.4243
 AVG MW                  18.0153    18.0153    28.0135    28.6277
71.9698

 S-321 S-322 S-323 S-324
 -----------------------

 STREAM ID               S-321      S-322      S-323      S-324
 FROM :                  F-302      V-301      F-302      P-302
 TO   :                  V-301      ----       P-302      ----

 SUBSTREAM: MIXED
 PHASE:                  MISSING    MISSING    LIQUID     LIQUID
 COMPONENTS: LBMOL/HR
   NITROGEN               0.0        0.0         0.1785     0.1785
   BETA--01               0.0        0.0         2.3649     2.3649
   ORTHO-01               0.0        0.0         0.0        0.0
   WATER                  0.0        0.0         1.8000     1.8000
   ACRYL-01               0.0        0.0       515.3845   515.3845
   P-MET-01               0.0        0.0         0.1000     0.1000
 TOTAL FLOW:
   LBMOL/HR               0.0        0.0       519.8279   519.8279
   LB/HR                  0.0        0.0      3.7361+04  3.7361+04
   CUFT/HR                0.0        0.0       580.0098   580.2043
 STATE VARIABLES:
   TEMP   F              MISSING    MISSING    100.0419   100.5996
   PRES   PSIA           15.0000    MISSING     15.0000    50.0000
   VFRAC                 MISSING    MISSING     0.0        0.0
   LFRAC                 MISSING    MISSING     1.0000     1.0000
   SFRAC                 MISSING    MISSING     0.0        0.0
 ENTHALPY:
   BTU/LBMOL             MISSING    MISSING -1.5627+05 -1.5626+05
   BTU/LB                MISSING    MISSING -2174.2925 -2174.1489
   BTU/HR                MISSING    MISSING -8.1233+07 -8.1228+07
 ENTROPY:
   BTU/LBMOL-R           MISSING    MISSING   -52.0947   -52.0905
   BTU/LB-R              MISSING    MISSING    -0.7248    -0.7248
 DENSITY:
   LBMOL/CUFT            MISSING    MISSING     0.8962     0.8959
```

LB/CUFT	MISSING	MISSING	64.4139	64.3923
AVG MW	MISSING	MISSING	71.8713	71.8713

APPENDIX F: MSDS

Refer to attached MSDS sheets



Health	2
Fire	4
Reactivity	0
Personal Protection	J

Material Safety Data Sheet
Acetaldehyde MSDS

Section 1: Chemical Product and Company Identification

Product Name: Acetaldehyde

Catalog Codes: SLA1309

CAS#: 75-07-0

RTECS: AB1925000

TSCA: TSCA 8(b) inventory: Acetaldehyde

CI#: Not applicable.

Synonym: Ethyl Aldehyde; Ethanal; Acetic Aldehyde

Chemical Name: Acetaldehyde

Chemical Formula: CH3CHO

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Acetaldehyde	75-07-0	100

Toxicological Data on Ingredients: Acetaldehyde: ORAL (LD50): Acute: 661 mg/kg [Rat.]. 900 mg/kg [Mouse]. DERMAL (LD50): Acute: 3540 mg/kg [Rabbit]. VAPOR (LC50): Acute: 13300 ppm 4 hours [Rat]. 23000 mg/m 4 hours [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation (lung irritant). Slightly hazardous in case of skin contact (irritant, permeator).

Potential Chronic Health Effects:
Hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (sensitizer). CARCINOGENIC EFFECTS: Classified 2B (Possible for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to liver. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 175°C (347°F) (ACGIH, 1996; Lewis, 1996; NFPA, 1994); 185 deg. C (ILO, 1998)

Flash Points:
CLOSED CUP: -38°C (-36.4°F) (Buvardi (1996); Clayton and Clayton, 1993; Lewis, 1996); -38.89 deg. C (American Conference of Govermental Industrial Hygienests) OPEN CUP: -40°C (-40°F) (Lewis, 1997; ACGIH, 1996 (Cleveland).

Flammable Limits:
LOWER: 4% UPPER: 55% (Clayton; Patty's Industrial Hygiene and Toxicology); 57% (American Conference of Govermental Industrial Hygiensts); 60% (National Fire Protection Association)

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances:
Extremely flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of static discharge: Not available. Explosive in presence of heat, of acids, of alkalis. Non-explosive in presence of shocks.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: When heated to decomposition it emits acrid smoke and fumes.

Special Remarks on Explosion Hazards:
Hazardous or explosive polymerization may occur with acids, alkaline materials, heat, strong bases, trace metals. Forms explosive peroxides on exposure to air, heat or sunlight.

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents, combustible materials, organic materials, metals, acids, alkalis.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves (impervious).

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 25 (ppm) from ACGIH (TLV) [United States] TWA: 200 STEL: 150 (ppm) from OSHA (PEL) [United States] TWA: 360 STEL: 270 (mg/m3) from OSHA (PEL) [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Fuming liquid.)

Odor: Fruity. Pungent. (Strong.)

Taste: Leafy green

Molecular Weight: 44.05 g/mole

Color: Colorless.

pH (1% soln/water): Not available.

Boiling Point: 21°C (69.8°F)

Melting Point: -123.5°C (-190.3°F)

Critical Temperature: 188°C (370.4°F)

Specific Gravity: 0.78 (Water = 1)

Vapor Pressure: 101.3 kPa (@ 20°C)

Vapor Density: 1.52 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.21 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:
Easily soluble in cold water, hot water. Soluble in diethyl ether, acetone. Miscible with benzene, gasoline, solvent naphtha, toluene, xylene, turpentine. Solubility in water: 1000 g/l @ 25 deg. C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, igition sources (flames, sparks), incompatible materials

Incompatibility with various substances:
Highly reactive with metals, acids, alkalis. Reactive with oxidizing agents, combustible materials, organic materials.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Reacts with oxidizing materials, halogens, amines, strong alkalies (bases), and acids, cobalt acetate, phenols, ketones, ammonia, hydrogen cyanide, hydrogen sulfide, hydrogen peroxide, mercury (II) salts (chlorate or perchlorate), acid anhydrides, alcohols, iodine, isocyanates, phosphorus, phosphorus isocyanate, tris(2-chlorobutyl)amine. It can slowly polymerize to paraldehyde. Polymerization may occur in presence of acid traces causing exothermic reaction, increased vessel pressure, fire, and explosion. Impure material polymerizes readily in presence of traces of metals (iron) or acids. Acetaldehyde is polymerized violently by concentrated sulfuric acid. Acetaldehyde can dissolve rubber.

Special Remarks on Corrosivity: Not available.

Polymerization: Not available.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 661 mg/kg [Rat.]. Acute dermal toxicity (LD50): 3540 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 23000 mg/m3 4 hours [Mouse].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified 2B (Possible for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Classified POSSIBLE for human. May cause damage to the following organs: liver.

Other Toxic Effects on Humans:
Hazardous in case of ingestion, of inhalation (lung irritant). Slightly hazardous in case of skin contact (irritant, permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and birth defects(teratogenic) based on animal test data May affect genetic material (mutagenic). May cause cancer based on animal test data

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes mild skin irritation. It can be absorbed through intact skin. Eyes: Causes severe eye irritation. Eye splashes produce painful but superficial corneal injuries which heal rapidly. Inhalation: It causes upper respiratory tract and mucous membrane irritation. It decreases the amount of pulmonary macrophages. It may cause bronchitis. It may cause pulmonary edema, often the cause of delayed death. It may affec respiration (dyspnea) and respiratory arrest and death may occur. It may affect behavior/central nervous and cause central nervous system depression. Iirritation usually prevents voluntary exposure to airborne concentrations high enough to cause CNS depression, although this effect has occurred in experimental animals. It may also affect the peripheral nervous system and cardiovascular system (hypotension or hypertension, tachycardia, bradycardia), kidneys (albuminuria) Chronic Potential Health Effects: Skin: Prolonged direct skin contact causes erythema and burns. Repeated exposure may cause dermatitis secondary to primary irritation or sensitization. Ingestion: Symptoms of chronic Acetaldehyde exposure may resemble those of chronic alcoholism. Acetaldehyde is the a metabolite of ethanol in humans and has been implicated as the active agent damaging the liver in ethanol-induced liver disease.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Acetaldehyde UNNA: 1089 PG: I

Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Acetaldehyde California prop. 65 (no significant risk level): Acetaldehyde: 0.09 mg/day (value) California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer which would require a warning under the statute: Acetaldehyde Connecticut hazardous material survey.: Acetaldehyde Illinois toxic substances disclosure to employee act: Acetaldehyde Illinois chemical safety act: Acetaldehyde New York release reporting list: Acetaldehyde Rhode Island RTK hazardous substances: Acetaldehyde Pennsylvania RTK: Acetaldehyde Minnesota: Acetaldehyde Massachusetts RTK: Acetaldehyde Massachusetts spill list: Acetaldehyde New Jersey: Acetaldehyde New Jersey spill list: Acetaldehyde New

Jersey toxic catastrophe prevention act: Acetaldehyde Louisiana spill reporting: Acetaldehyde California Director's List of Hazardous Substances: Acetaldehyde TSCA 8(b) inventory: Acetaldehyde SARA 313 toxic chemical notification and release reporting: Acetaldehyde CERCLA: Hazardous substances.: Acetaldehyde: 1000 lbs. (453.6 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R12- Extremely flammable. R36/37/38- Irritating to eyes, respiratory system and skin. R40- Possible risks of irreversible effects. S16- Keep away from sources of ignition - No smoking. S33- Take precautionary measures against static discharges. S36/37/39- Wear suitable protective clothing, gloves and eye/face protection.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 4

Reactivity: 0

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 4

Reactivity: 2

Specific hazard:

Protective Equipment:
Gloves (impervious). Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Liste des produits purs tératogènes, mutagènes, cancérogènes. Répertoire toxicologique de la Commission de la Santé et de la Sécurité du Travail du Québec. -Material safety data sheet emitted by: la Commission de la Santé et de la Sécurité du Travail du Québec. -SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -Guide de la loi et du règlement sur le transport des marchandises dangeureuses au canada. Centre de conformité internatinal Ltée. 1986.

Other Special Considerations: Not available.

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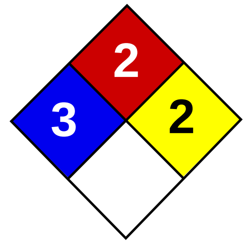
Last Updated: 05/21/2013 12:00 PM



Health	3
Fire	2
Reactivity	2
Personal Protection	

Material Safety Data Sheet
Acrylic Acid MSDS

Section 1: Chemical Product and Company Identification

Product Name: Acrylic Acid

Catalog Codes: SLA3406

CAS#: 79-10-7

RTECS: AS4375000

TSCA: TSCA 8(b) inventory: Acrylic Acid

CI#: Not available.

Synonym: Propenoic Acid Ethylenecarboxylic Acid

Chemical Name: Acrylic Acid

Chemical Formula: C3-H4-O2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Acrylic Acid	79-10-7	100

Toxicological Data on Ingredients: Acrylic Acid: ORAL (LD50): Acute: 33500 mg/kg [Rat]. 2400 mg/kg [Mouse]. DERMAL (LD50): Acute: 294 mg/kg [Rabbit]. VAPOR (LC50): Acute: 5300 mg/m 2 hours [Mouse]. 75 ppm 6 hours [Monkey].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (permeator), of eye contact (irritant, corrosive). Corrosive to skin and eyes on contact. Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth and respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation of respiratory tract, characterized by coughing, choking, or shortness of breath. Severe over-exposure can result in death. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian germ and somatic cells. TERATOGENIC EFFECTS: Classified SUSPECTED for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. Classified Development toxin [SUSPECTED]. The substance is toxic to bladder, brain, upper respiratory tract, eyes, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged contact with spray mist may produce chronic eye irritation and severe skin irritation.

Repeated or prolonged exposure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection. Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 438°C (820.4°F)

Flash Points: CLOSED CUP: 50°C (122°F).

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO_2).

Fire Hazards in Presence of Various Substances:
Extremely flammable in presence of open flames and sparks. Highly flammable in presence of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.

Large Spill:
Flammable liquid. Corrosive liquid. Poisonous liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use water spray curtain to divert vapor drift. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Never add water to this product. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids, alkalis, moisture.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Face shield. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Boots.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 2 (ppm) from ACGIH (TLV) [United States] [1997] TWA: 2 [Australia] STEL: 20 (ppm) [United Kingdom (UK)] TWA: 10 (ppm) [United Kingdom (UK)] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Acrid (Strong.)

Taste: Not available.

Molecular Weight: 72.06 g/mole

Color: Colorless.

pH (1% soln/water): Not available.

Boiling Point: 141°C (285.8°F)

Melting Point: 14°C (57.2°F)

Critical Temperature: 342°C (647.6°F)

Specific Gravity: 1.05 (Water = 1)

Vapor Pressure: 0.5 kPa (@ 20°C)

Vapor Density: 2.5 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.092 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 0.4

Ionicity (in Water): Not available.

Dispersion Properties:
Partially dispersed in methanol, diethyl ether. See solubility in water.

Solubility:
Soluble in cold water. Very slightly soluble in acetone. Insoluble in diethyl ether.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances:
Extremely reactive or incompatible with oxidizing agents, acids, alkalis. Reactive with moisture.

Corrosivity:
Slightly corrosive in presence of steel, of aluminum, of zinc, of copper. Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Yes.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 2400 mg/kg [Mouse]. Acute dermal toxicity (LD50): 294 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 75 6 hours [Monkey].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian germ and somatic cells. TERATOGENIC EFFECTS: Classified SUSPECTED for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. Classified Development toxin [SUSPECTED]. Causes damage to the following organs: bladder, brain, upper respiratory tract, eyes, central nervous system (CNS).

Other Toxic Effects on Humans:
Very hazardous in case of skin contact (permeator), of eye contact (corrosive). Hazardous in case of skin contact (corrosive), of inhalation (lung corrosive).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 130 mg/l 24 hours [Trout]. 460 mg/l 96 hours [Trout]. 270 mg/l 24 hours [Water flea].

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

Identification: : Acrylic Acid, Inhibited UNNA: UN2218 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Rhode Island RTK hazardous substances: Acrylic Acid Pennsylvania RTK: Acrylic Acid Florida: Acrylic Acid Minnesota: Acrylic Acid Massachusetts RTK: Acrylic Acid New Jersey: Acrylic Acid TSCA 8(b) inventory: Acrylic Acid TSCA 5(e) substance consent order: Acrylic Acid TSCA 8(a) IUR: Acrylic Acid TSCA 12(b) annual export notification: Acrylic Acid SARA 313 toxic chemical notification and release reporting: Acrylic Acid CERCLA: Hazardous substances.: Acrylic Acid: 1 lbs. (0.4536 kg)

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). CLASS E: Corrosive liquid.

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 2

Reactivity: 2

Personal Protection:

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 2

Reactivity: 2

Specific hazard:

Protective Equipment:
Gloves. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Face shield.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 05/21/2013 12:00 PM

Science Lab.com
Chemicals & Laboratory Equipment

Health	0
Fire	2
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
beta-Propiolactone MSDS

Section 1: Chemical Product and Company Identification

Product Name: beta-Propiolactone

Catalog Codes: SLP4486

CAS#: 57-57-8

RTECS: RQ7350000

TSCA: TSCA 8(b) inventory: beta-Propiolactone

CI#: Not available.

Synonym: 2-Oxetanone

Chemical Formula: C3H4O2

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{beta-}Propiolactone	57-57-8	100

Toxicological Data on Ingredients: beta-Propiolactone: VAPOR (LC50): Acute: 25 ppm 4 hour(s) [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of ingestion, of inhalation. Hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator). Corrosive to skin and eyes on contact. Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth and respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation of respiratory tract, characterized by coughing, choking, or shortness of breath. Severe over-exposure can result in death.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Classified + (PROVEN) by OSHA. Classified 2B (Possible for human.) by IARC. Classified A2 (Suspected for human.) by ACGIH, 2 (Reasonably anticipated.) by NTP. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to kidneys, lungs, liver, digestive system. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged contact with spray mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged exposure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection. Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
If the chemical got onto the clothed portion of the body, remove the contaminated clothes as quickly as possible, protecting your own hands and body. Place the victim under a deluge shower. If the chemical got on the victim's exposed skin, such as the hands : Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cold water may be used. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Combustible.

Auto-Ignition Temperature: Not available.

Flash Points: OPEN CUP: 70°C (158°F).

Flammable Limits: LOWER: 2.9%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Flammable in presence of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.

Large Spill:
Combustible material. Corrosive liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up Keep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. Never add water to this product Wear suitable protective clothing In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 0.5 (ppm) TWA: 1.5 (mg/m3) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Pungent.

Taste: Not available.

Molecular Weight: 72.06 g/mole

Color: Colorless.

pH (1% soln/water): Not available.

Boiling Point: Decomposes. (155°C or 311°F)

Melting Point: -33.4°C (-28.1°F)

Critical Temperature: Not available.

Specific Gravity: 1.48 (Water = 1)

Vapor Pressure: 3.4 mm of Hg (@ 20°C)

Vapor Density: 2.5 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility: Soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Yes.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute toxicity of the vapor (LC50): 25 ppm 4 hour(s) [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified + (PROVEN) by OSHA. Classified 2B (Possible for human.) by IARC. Classified A2 (Suspected for human.) by ACGIH, 2 (Reasonably anticipated.) by NTP. The substance is toxic to kidneys, lungs, liver, digestive system.

Other Toxic Effects on Humans:
Very hazardous in case of ingestion, of inhalation. Hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 6.1: Poisonous material.

Identification: : Toxic liquids n.o.s. : UN2810 PG: Not available.

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: beta-Propiolactone California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer which would require a warning under the statute: beta-Propiolactone Pennsylvania RTK: beta-Propiolactone Florida: beta-Propiolactone Minnesota: beta-Propiolactone Massachusetts RTK: beta-Propiolactone New Jersey: beta-Propiolactone TSCA 8(b) inventory: beta-Propiolactone SARA 313 toxic chemical notification and release reporting: beta-Propiolactone CERCLA: Hazardous substances.: beta-Propiolactone

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). CLASS D-1A: Material causing immediate and serious toxic effects (VERY TOXIC). CLASS D-2A: Material causing other toxic effects (VERY TOXIC). CLASS E: Corrosive liquid.

DSCL (EEC):
R26- Very toxic by inhalation. R36/38- Irritating to eyes and skin. R45- May cause cancer.

HMIS (U.S.A.):

Health Hazard: 0

Fire Hazard: 2

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 0

Flammability: 2

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/09/2005 06:12 PM

Last Updated: 05/21/2013 12:00 PM

Material Safety Data Sheet

Carbon Monoxide

Section 1. Chemical product and company identification

Product name	:	Carbon Monoxide
Supplier	:	AIRGAS INC., on behalf of its subsidiaries 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
Product use	:	Synthetic/Analytical chemistry.
Synonym	:	Carbon oxide (CO); CO; Exhaust Gas; Flue gas; Carbonic oxide; Carbon oxide; Carbone; Carbonio; Kohlenmonoxid; Kohlenoxyd; Koolmonoxyde; NA 9202; Oxyde de carbone; UN 1016; Wegla tlenek; Flue gasnide; Carbon monooxide
MSDS #	:	001014
Date of Preparation/Revision	:	**12/3/2012.**
In case of emergency	:	1-866-734-3438

Section 2. Hazards identification

Physical state	:	Gas. [[COLORLESS GAS, MAY BE A LIQUID AT LOW TEMPERATURE OR HIGH PRESSURE.]]
Emergency overview	:	WARNING! FLAMMABLE GAS. MAY CAUSE FLASH FIRE. MAY BE FATAL IF INHALED. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA. CONTENTS UNDER PRESSURE. Keep away from heat, sparks and flame. Do not puncture or incinerate container. Avoid breathing gas. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed. Contact with rapidly expanding gases can cause frostbite.
Target organs	:	May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).
Routes of entry	:	Inhalation

Potential acute health effects

Eyes	:	Contact with rapidly expanding gas may cause burns or frostbite.
Skin	:	Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation	:	Toxic by inhalation.
Ingestion	:	Ingestion is not a normal route of exposure for gases

Potential chronic health effects

Chronic effects	:	May cause target organ damage, based on animal data.
Target organs	:	May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).
Medical conditions aggravated by over-exposure	:	Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Carbon Monoxide	630-08-0	100	**ACGIH TLV (United States, 2/2010).** TWA: 29 mg/m³ 8 hour(s). TWA: 25 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 10 hour(s). TWA: 35 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 55 mg/m³ 8 hour(s). TWA: 50 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 8 hour(s). TWA: 35 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 605°C (1121°F)

Flammable limits : Lower: 12.5% Upper: 74.2%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances : Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

Product name

carbon monoxide	**ACGIH TLV (United States, 2/2010).** TWA: 29 mg/m³ 8 hour(s). TWA: 25 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 229 mg/m³ CEIL: 200 ppm TWA: 40 mg/m³ 10 hour(s). TWA: 35 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 55 mg/m³ 8 hour(s).

TWA: 50 ppm 8 hour(s).
OSHA PEL 1989 (United States, 3/1989).
CEIL: 229 mg/m³
CEIL: 200 ppm
TWA: 40 mg/m³ 8 hour(s).
TWA: 35 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 28.01 g/mole
Molecular formula : C-O
Boiling/condensation point : -191°C (-311.8°F)
Melting/freezing point : -205°C (-337°F)
Critical temperature : -140.1°C (-220.2°F)
Vapor density : 0.97 (Air = 1)
Specific Volume (ft ^{3}/lb) : 13.8889
Gas Density (lb/ft ^{3}) : 0.072

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	Result	Species	Dose	Exposure
carbon monoxide	TDLo Intraperitoneal	Rat	35 mL/kg	-
	LC50 Inhalation Vapor	Rat	13500 mg/m3	15 minutes
	LC50 Inhalation Vapor	Rat	1900 mg/m3	4 hours
	LC50 Inhalation Gas.	Rat	6600 ppm	30 minutes
	LC50 Inhalation Gas.	Rat	3760 ppm	1 hours
	LC50 Inhalation Gas.	Mouse	2444 ppm	4 hours
	LC50 Inhalation Gas.	Rat	1807 ppm	4 hours

IDLH : 1200 ppm
Chronic effects on humans : **TERATOGENIC EFFECTS**: Classified 1 by European Union.
May cause damage to the following organs: blood, lungs, the nervous system, heart, cardiovascular system, central nervous system (CNS).
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Not available.

Products of degradation	:	Products of degradation: carbon oxides (CO, CO_2).
Environmental fate	:	Not available.
Environmental hazards	:	No known significant effects or critical hazards.
Toxicity to the environment	:	Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).	 	Inhalation hazard zone D **Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 25 kg **Special provisions** 4
TDG Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).	 	**Explosive Limit and Limited Quantity Index** 0 **ERAP Index** 500 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index**

						Forbidden
Mexico Classification	UN1016	CARBON MONOXIDE, COMPRESSED	2.3	Not applicable (gas).	 	-

“Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.”

Section 15. Regulatory information

United States

U.S. Federal regulations : **TSCA 8(a) IUR**: Not determined
United States inventory (TSCA 8b): This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: carbon monoxide
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: carbon monoxide: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard

State regulations : **Connecticut Carcinogen Reporting**: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

California Prop. 65 : **WARNING:** This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

Ingredient name	Cancer	Reproductive	No significant risk level	Maximum acceptable dosage level
Carbon Monoxide	No.	Yes.	No.	No.

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

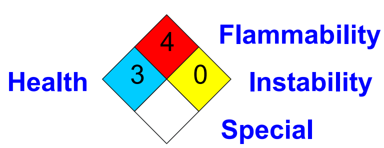
Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).

Hazardous Material Information System (U.S.A.) :

Health	*	2
Flammability		4
Physical hazards		0

National Fire Protection Association (U.S.A.) :



Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Material Safety Data Sheet
Dicobalt octacarbonyl

ACC# 56919

Section 1 - Chemical Product and Company Identification

MSDS Name: Dicobalt octacarbonyl
Catalog Numbers: AC291840000, AC291840050, AC291840250
Synonyms: Cobalt carbonyl; Cobalt tetracarbonyl dimer.
Company Identification:

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01
For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
10210-68-1	Cobalt carbonyl	95	233-514-0
110-54-3	Hexane	5	203-777-6

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: dark orange solid.
Danger! Pyrophoric. Spontaneously flammable in air. May be pyrophoric and become spontaneously flammable in air. May cause allergic respiratory and skin reaction. May be harmful if swallowed. Air sensitive.
Target Organs: Lungs, skin.

Potential Health Effects
Eye: May cause eye irritation.
Skin: May cause skin irritation. May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material.
Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed.

Inhalation: May cause respiratory tract irritation. Inhalation of fumes may cause metal fume fever, which is characterized by flu-like symptoms with metallic taste, fever, chills, cough, weakness, chest pain, muscle pain and increased white blood cell count. In rare instances, exposure may cause sensitization, resulting in inflammation of the mucous membranes and in eczematous eruptions.
Chronic: May cause kidney injury. Cobalt compounds may cause cancer based upon animal studies.

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.
Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.
Ingestion: If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately.
Inhalation: Get medical aid immediately. Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Do NOT use mouth-to-mouth resuscitation.
Notes to Physician: Treat symptomatically and supportively.
Antidote: There exists several chelation agents. The determination of there use should be made only by qualified medical personnel.

Section 5 - Fire Fighting Measures

General Information: Evacuate area and fight fire from a safe distance. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. May burn with invisible flame. Water reactive. Material will react with water and may release a flammable and/or toxic gas. Use water spray to keep fire-exposed containers cool. Spontaneously ignitable in air. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas. May burn rapidly with flare burning effect. May re-ignite after fire is extinguished. Containers may explode if exposed to fire.
Extinguishing Media: Do NOT use water directly on fire. Do NOT get water inside containers. Contact professional fire-fighters immediately. Cool containers with flooding quantities of water until well after fire is out. For small fires, use dry chemical, soda ash, lime or sand. For large fires, use dry sand, dry chemical, soda ash or lime or withdraw from area and let fire burn.
Flash Point: Not available.
Autoignition Temperature: Not available.
Explosion Limits, Lower:N/A
Upper: N/A
NFPA Rating: (estimated) Health: 2; Flammability: 2; Instability: 2; Special Hazard: -W-

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Clean up spills immediately, observing precautions in the Protective Equipment section. Sweep up or absorb material, then place into a suitable clean, dry, closed container for disposal. Isolate area and deny entry. Place under an inert atmosphere. Do not use combustible materials such as paper towels to clean up spill.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Use only in a well-ventilated area. Minimize dust generation and accumulation. Use spark-proof tools and explosion proof equipment. Avoid contact with eyes, skin, and clothing. Avoid contact with skin and eyes. Avoid ingestion and inhalation. Handle under an inert atmosphere. Store protected from air.
Storage: Keep away from heat, sparks, and flame. Store in a cool, dry place. Keep away from water. Refrigerator/flammables. Keep containers tightly closed. Do not expose to air. Store under an inert atmosphere.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use explosion-proof ventilation equipment. Use adequate ventilation to keep airborne concentrations low.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Cobalt carbonyl	0.1 mg/m3 TWA (as Co)	0.1 mg/m3 TWA (as Co)	none listed
Hexane	50 ppm TWA; Skin - potential significant contribution to overall exposure by the cutaneous r oute	50 ppm TWA; 180 mg/m3 TWA 1100 ppm IDLH	500 ppm TWA; 1800 mg/m3 TWA

OSHA Vacated PELs: Cobalt carbonyl: 0.1 mg/m3 TWA (as Co) Hexane: 50 ppm TWA; 180 mg/m3 TWA
Personal Protective Equipment
Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard

EN166.
Skin: Wear appropriate gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to minimize contact with skin.
Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use. Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Solid
Appearance: dark orange
Odor: none reported
pH: Not available.
Vapor Pressure: Not available.
Vapor Density: 12.0
Evaporation Rate: Not available.
Viscosity: Not available.
Boiling Point: 52 deg C
Freezing/Melting Point:51.00 - 52.00 deg C
Decomposition Temperature:> 52 deg C
Solubility: insoluble
Specific Gravity/Density:1.8100g/cm3
Molecular Formula:$C_8Co_2O_8$
Molecular Weight:341.8616

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures. Powder or liquid is pyrophoric.
Conditions to Avoid: Incompatible materials, ignition sources, dust generation, exposure to air, strong oxidants.
Incompatibilities with Other Materials: Strong oxidizing agents.
Hazardous Decomposition Products: Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, oxides of cobalt.
Hazardous Polymerization: Has not been reported

Section 11 - Toxicological Information

RTECS#:
CAS# 10210-68-1: GG0300000
CAS# 110-54-3: MN9275000
LD50/LC50:
CAS# 10210-68-1:
    Inhalation, mouse: LC50 = 26900 ug/m3/2H;
    Inhalation, rat: LC50 = 165 mg/m3;
    Oral, mouse: LD50 = 378 mg/kg;
    Oral, rat: LD50 = 754 mg/kg;
.

CAS# 110-54-3:
    Draize test, rabbit, eye: 10 mg Mild;
    Inhalation, mouse: LC50 = 150000 mg/m3/2H;
    Inhalation, rat: LC50 = 48000 ppm/4H;
    Inhalation, rat: LC50 = 627000 mg/m3/3M;
    Oral, rat: LD50 = 25 gm/kg;
.

Carcinogenicity:
CAS# 10210-68-1:

- **ACGIH:** Not listed.
- **California:** Not listed.
- **NTP:** Not listed.
- **IARC:** Group 2B carcinogen

CAS# 110-54-3: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No data available.
Teratogenicity: No data available.
Reproductive Effects: No data available.
Mutagenicity: No data available.
Neurotoxicity: No data available.
Other Studies:

Section 12 - Ecological Information

No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste

regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	DOT regulated - small quantity provisions apply (see 49CFR173.4)	FLAMMABLE SOLID ORGANIC NOS (DICOBALT OCTACARBONYL)
Hazard Class:		4.1
UN Number:		UN1325
Packing Group:		II

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 10210-68-1 is listed on the TSCA inventory.
CAS# 110-54-3 is listed on the TSCA inventory.
Health & Safety Reporting List
None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
CAS# 110-54-3: 5000 lb final RQ; 2270 kg final RQ
SARA Section 302 Extremely Hazardous Substances
CAS# 10210-68-1: 10 lb TPQ (lower threshold); 10000 lb TPQ (upper thre shold)
SARA Codes
CAS # 110-54-3: immediate, delayed, fire.
Section 313
This material contains Cobalt carbonyl (listed as Cobalt compounds), 95%, (CAS# 10210-68-1) which is subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.
This material contains Hexane (CAS# 110-54-3, 5%),which is subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.
Clean Air Act:
CAS# 10210-68-1 (listed as Cobalt compounds) is listed as a hazardous air pollutant

(HAP).

CAS# 110-54-3 is listed as a hazardous air pollutant (HAP).

This material does not contain any Class 1 Ozone depletors.

This material does not contain any Class 2 Ozone depletors.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 10210-68-1 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.

CAS# 110-54-3 can be found on the following state right to know lists: New Jersey, Pennsylvania, Minnesota, Massachusetts.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

T+ F

Risk Phrases:

R 11 Highly flammable.

R 22 Harmful if swallowed.

R 42/43 May cause sensitization by inhalation and skin contact.

Safety Phrases:

S 16 Keep away from sources of ignition - No smoking.

S 24/25 Avoid contact with skin and eyes.

WGK (Water Danger/Protection)

CAS# 10210-68-1: No information available.

CAS# 110-54-3: 1

Canada - DSL/NDSL

CAS# 10210-68-1 is listed on Canada's DSL List.

CAS# 110-54-3 is listed on Canada's DSL List.

Canada - WHMIS

This product has a WHMIS classification of B4.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

CAS# 10210-68-1 is listed on the Canadian Ingredient Disclosure List.

CAS# 110-54-3 is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 5/01/1998
Revision #5 Date: 6/21/2006

Material Safety Data Sheet

Ethylene Oxide

Section 1. Chemical product and company identification

Product name : Ethylene Oxide

Supplier : AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use : Synthetic/Analytical chemistry.

Synonym : Oxirane; Dihydrooxirene; Dimethylene oxide; Epoxyethane; Ethene oxide; ETO; Oxacyclopropane; Oxane; Oxidoethane; Oxirene, Dihydro-; Oxyfume; Oxyfume 12; T-Gas; 1,2-Epoxyethane; Aethylenoxid; Amprolene; Anprolene; Anproline; ENT-26263; E.O.; 1,2-Epoxyaethan; Ethox; Ethyleenoxide; Etylenu tlenek; FEMA No. 2433; Merpol; NCI-C50088; α,β-Oxidoethane; Oxiraan; Oxiran; Rcra waste number U115; Sterilizing gas ethylene oxide 100%; UN 1040; C2H4O; Qazi-ketcham

MSDS # : 001081

Date of Preparation/Revision : **4/19/2012.**

In case of emergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS GAS AT ROOM TEMP. MOBILE LIQUID BELOW BOILING POINT. HAS A SWEET ODOR]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
HARMFUL IF INHALED OR SWALLOWED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CANCER HAZARD - CAN CAUSE CANCER.
CAUSES SEVERE SKIN IRRITATION.
CAUSES SEVERE EYE IRRITATION.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Do not ingest. Avoid breathing gas. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Risk of cancer depends on duration and level of exposure. Use only with adequate ventilation. Wash thoroughly after handling. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: blood, kidneys, lungs, the reproductive system, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

Routes of entry : Inhalation Dermal Eyes

Potential acute health effects

Eyes : Severely irritating to eyes. Risk of serious damage to eyes. Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Severely irritating to the skin. Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Toxic by inhalation.

Ingestion : Ingestion is not a normal route of exposure for gases

Potential chronic health effects

Carcinogenicity : Can cause cancer. Risk of cancer depends on duration and level of exposure.

Target organs : May cause damage to the following organs: blood, kidneys, lungs, the reproductive system, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

Medical conditions aggravated by over-exposure : Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CAS number	% Volume	Exposure limits
Ethylene Oxide	75-21-8	100	**ACGIH TLV (United States, 1/2009).** TWA: 1.8 mg/m³ 8 hour(s). TWA: 1 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 9 mg/m³ 10 minute(s). CEIL: 5 ppm TWA: 0.18 mg/m³ 10 hour(s). TWA: 0.1 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** STEL: 5 ppm 15 minute(s). TWA: 1 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 5 ppm 15 minute(s). TWA: 1 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training.If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus.It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact : Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact : In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite : Try to warm up the frozen tissues and seek medical attention.

Inhalation : Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion : As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 428.88°C (804°F)

Flash point : Open cup: -29.15°C (-20.5°F).

Flammable limits : Lower: 3% Upper: 100%

Products of combustion : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire-fighting media and instructions : In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions : Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling : Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Wash thoroughly after handling. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Do not ingest. Keep container closed. Avoid contact with skin and clothing. Avoid contact with eyes. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage : Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

Product name

Ethylene Oxide	
ethylene oxide	**ACGIH TLV (United States, 1/2009).** TWA: 1.8 mg/m³ 8 hour(s). TWA: 1 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** CEIL: 9 mg/m³ 10 minute(s). CEIL: 5 ppm TWA: 0.18 mg/m³ 10 hour(s). TWA: 0.1 ppm 10 hour(s). **OSHA PEL (United States, 11/2006).** STEL: 5 ppm 15 minute(s). TWA: 1 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** STEL: 5 ppm 15 minute(s). TWA: 1 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight : 44.06 g/mole

Molecular formula : C2-H4-O

Boiling/condensation point : 10.7°C (51.3°F)

Melting/freezing point : -112.8°C (-171°F)

Critical temperature : 195.9°C (384.6°F)

Vapor pressure : 22 (psia)

Vapor density : 1.52 (Air = 1)

Specific Volume (ft ^{3}/lb) : 8.7719

Gas Density (lb/ft ^{3}) : 0.114

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Product/ingredient name	Result	Species	Dose	Exposure
ethylene oxide	LD50 Oral	Rat	72 mg/kg	-
	LD50 Subcutaneous	Rat	187 mg/kg	-
	LDLo Unreported	Rat	200 mg/kg	-
	LC50 Inhalation Gas.	Rat	1460 ppm	4 hours
	LC50 Inhalation Gas.	Mouse	836 ppm	4 hours
	LC50 Inhalation Gas.	Rat	800 ppm	4 hours
	LC50 Inhalation Gas.	Rat	800 ppm	4 hours

IDLH : 800 ppm

Chronic effects on humans : **CARCINOGENIC EFFECTS**: Classified 1 (Proven for humans.) by IARC, 1 (Known to be human carcinogens.) by NTP, + (Proven.) by OSHA, + (Proven.) by NIOSH. Classified A2 (Suspected for humans.) by ACGIH, 2 (Suspected for humans.) by European Union.
MUTAGENIC EFFECTS: Classified 2 by European Union.
May cause damage to the following organs: blood, kidneys, lungs, the reproductive system, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

Other toxic effects on humans : Hazardous by the following route of exposure: of skin contact (irritant), of eye contact (irritant), of inhalation (lung irritant).

Specific effects

Carcinogenic effects : Can cause cancer. Risk of cancer depends on duration and level of exposure.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

Product/ingredient name	Test	Result	Species	Exposure
ethylene oxide	-	Acute LC50 1000000 ug/L Marine water	Crustaceans - Brine shrimp - Artemia sp.	48 hours
	-	Acute LC50 >500000 ug/L Marine water	Crustaceans - Brine shrimp - Artemia sp.	48 hours
	-	Acute LC50 490000 ug/L Marine water	Crustaceans - Brine shrimp - Artemia sp.	48 hours
	-	Acute LC50 300000 ug/L Fresh water	Daphnia - Water flea - Daphnia magna	48 hours
	-	Acute LC50 200000 to 243000 ug/L Fresh water	Daphnia - Water flea - Daphnia magna	48 hours
	-	Acute LC50 137000 to 179000 ug/L Fresh water	Daphnia - Water flea - Daphnia magna	48 hours
	-	Acute LC50 84000 to 96000 ug/L Fresh water	Fish - Fathead minnow - Pimephales promelas	96 hours

Products of degradation :

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

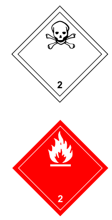
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation.Return cylinders with residual product to Airgas, Inc.Do not dispose of locally.

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information

Ethylene Oxide						
DOT Classification	UN1040	Ethylene Oxide	2.3	Not applicable (gas).		**Reportable quantity** 10 lbs. (4.54 kg)
TDG Classification	UN1040	Ethylene Oxide	2.3	Not applicable (gas).		**Explosive Limit and Limited Quantity Index** 0 **ERAP Index** 500 **Passenger Carrying Ship Index** Forbidden **Passenger Carrying Road or Rail Index** Forbidden
Mexico Classification	UN1040	Ethylene Oxide	2.3	Not applicable (gas).		-

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations : **United States inventory (TSCA 8b):** This material is listed or exempted.

SARA 302/304/311/312 extremely hazardous substances: ethylene oxide
SARA 302/304 emergency planning and notification: ethylene oxide
SARA 302/304/311/312 hazardous chemicals: ethylene oxide
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: ethylene oxide: Fire hazard, reactive, Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard

Clean Water Act (CWA) 307: No products were found.

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

Clean Air Act (CAA) 112 regulated toxic substances: ethylene oxide

SARA 313

	Product name	CAS number	Concentration
Form R - Reporting requirements :	Ethylene Oxide	75-21-8	100

Supplier notification : Ethylene Oxide 75-21-8 100

SARA 313 notifications must not be detached from the MSDS and any copying and redistribution of the MSDS shall include copying and redistribution of the notice attached to copies of the MSDS subsequently redistributed.

State regulations :
Connecticut Carcinogen Reporting: This material is not listed.
Connecticut Hazardous Material Survey: This material is not listed.
Florida substances: This material is not listed.
Illinois Chemical Safety Act: This material is not listed.
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
Louisiana Reporting: This material is not listed.
Louisiana Spill: This material is not listed.
Massachusetts Spill: This material is not listed.
Massachusetts Substances: This material is listed.
Michigan Critical Material: This material is not listed.
Minnesota Hazardous Substances: This material is not listed.
New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is listed.
New York Acutely Hazardous Substances: This material is listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

California Prop. 65 : **WARNING:** This product contains a chemical known to the State of California to cause cancer and birth defects or other reproductive harm.

Ingredient name	Cancer	Reproductive	No significant risk level	Maximum acceptable dosage level
Ethylene Oxide	Yes.	Yes.	Yes.	Yes.

Canada

WHMIS (Canada) :
Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).
Class E: Corrosive material
Class F: Dangerously reactive material.

CEPA Toxic substances: This material is listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States

Label requirements :
FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
HARMFUL IF INHALED OR SWALLOWED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CANCER HAZARD - CAN CAUSE CANCER.
CAUSES SEVERE SKIN IRRITATION.
CAUSES SEVERE EYE IRRITATION.
CONTENTS UNDER PRESSURE.

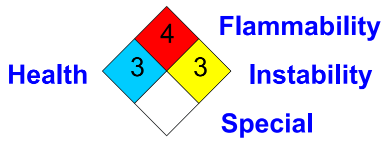
Canada

Label requirements :
Class A: Compressed gas.
Class B-1: Flammable gas.
Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
Class D-2A: Material causing other toxic effects (Very toxic).
Class E: Corrosive material
Class F: Dangerously reactive material.

Hazardous Material Information System (U.S.A.) :

Health	*	3
Flammability		4
Physical hazards		3

National Fire Protection Association (U.S.A.) :



Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

ScienceLab.com
Chemicals & Laboratory Equipment

Health	3
Fire	2
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Monoethanolamine MSDS

Section 1: Chemical Product and Company Identification

Product Name: Monoethanolamine

Catalog Codes: SLA4792, SLA2452, SLA3955

CAS#: 141-43-5

RTECS: KJ5775000

TSCA: TSCA 8(b) inventory: Ethanolamine

CI#: Not applicable.

Synonym: Colamine, Glycinol, Olamine; Ethanolamine; 2-Aminoethanol; 2-Hydroxyethylamine; beta-Ethanolamine; beta-Hydroxyethylamine

Chemical Name: Ethanol 2-amino

Chemical Formula: HOCH2CH2NH2 or C2-H7-N-O

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Ethanolamine	141-43-5	100

Toxicological Data on Ingredients: Ethanolamine: ORAL (LD50): Acute: 1720 mg/kg [Rat.]. 700 mg/kg [Mouse]. DERMAL (LD50): Acute: 1000 mg/kg [Rabbit.].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of ingestion, . Hazardous in case of skin contact (irritant, permeator), of inhalation (lung irritant). Slightly hazardous in case of skin contact (corrosive), of eye contact (corrosive). Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth and respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation of respiratory tract, characterized by coughing, choking, or shortness of breath. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to kidneys, lungs, liver, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged contact with spray mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged exposure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention immediately. Finish by rinsing thoroughly with running water to avoid a possible infection.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Combustible.

Auto-Ignition Temperature: 410°C (770°F)

Flash Points: CLOSED CUP: 86°C (186.8°F). OPEN CUP: 93.34°C (200°F) (Cleveland).

Flammable Limits: LOWER: 3% UPPER: 23.5%

Products of Combustion: These products are carbon oxides (CO, CO_2), nitrogen oxides (NO, NO_2...).

Fire Hazards in Presence of Various Substances:
Flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:

Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container. If necessary: Neutralize the residue with a dilute solution of acetic acid.

Large Spill:
Combustible material. Corrosive liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of acetic acid. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers. Hygroscopic

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Face shield. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Boots.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 3 STEL: 5 (ppm) [United Kingdom (UK)] TWA: 3 STEL: 6 (ppm) from ACGIH (TLV) [United States] STEL: 15 (mg/m3) from NIOSH [United States] TWA: 3 STEL: 6 (ppm) from NIOSH [United States] TWA: 3 (ppm) from OSHA (PEL) [United States] TWA: 6 (mg/m3) from OSHA (PEL) [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Viscous liquid.)

Odor: Ammoniacal. Fish. Unpleasant.

Taste: Not available.

Molecular Weight: 61.08 g/mole

Color: Colorless. Clear

pH (1% soln/water): 10 [Basic.]

Boiling Point: 170.8°C (339.4°F)

Melting Point: 10.3°C (50.5°F)

Critical Temperature: 341°C (645.8°F)

Specific Gravity: 1.018 (Water = 1)

Vapor Pressure: 0.1 kPa (@ 20°C)

Vapor Density: 2.1 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -1.3

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, methanol, diethyl ether, acetone.

Solubility:
Soluble in cold water, hot water, methanol, acetone. Partially soluble in diethyl ether. Solubility in Benzene @ 25 deg. C: 1.4% Solubility in Ether: 2.1% Solubility in Carbon Tetrachloride: 0.2% Solubility in Heptane: <0.1% Miscible with Chloroform, Glycerin. Immiscible with fixed oils, solvent Hexane. Slightly soluble in Petroleum Ether.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, incompatible materials, light, moisture

Incompatibility with various substances: Reactive with oxidizing agents, acids.

Corrosivity: Highly corrosive in presence of aluminum, of copper.

Special Remarks on Reactivity:
Hygroscopic; keep container tightly closed. Sensitive to light. INCOMPATIBLE WITH: ACETIC ACID, ACETIC ANHYDRIDE, ACROLEIN, ACRYLIC ACID, ACRYLONITRILE, CHLOROSULFONIC ACID, EPICHLOROHYDRIN, HYDROCHLORIC ACID, HYDROFLUORIC ACID, MESITYL OXIDE, NITRIC ACID, OLEUM, PROPIOLACTONE (BETA-), SULFURIC ACID, VINYL ACETATE, HALOGENS.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 700 mg/kg [Mouse]. Acute dermal toxicity (LD50): 1000 mg/kg [Rabbit.].

Chronic Effects on Humans: May cause damage to the following organs: kidneys, lungs, liver, central nervous system (CNS).

Other Toxic Effects on Humans:
Very hazardous in case of ingestion, . Hazardous in case of skin contact (irritant, permeator), of inhalation (lung irritant). Slightly hazardous in case of skin contact (corrosive), of eye contact (corrosive).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and birth defects (teratogenic) based on animal test data. May affect genetic material (mutagenic)

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: Skin: Causes moderate skin irritation and possible burns. It can be absorbed through the skin. It may be harmful if absorbed through the skin. Eyes: Causes severe eye irritation and possible eye burns. Inhalation: Causes respiratory tract irritation. May cause shortness of breath and an asthma-like condition. It may also affect behavior/ central nervous system (nausea, headache, weakness, dizziness, giddiness, sleepiness, loss of coordination and jugdement) Ingestion: May be harmful if swallowed. Causes gastrointestinal tract irritation with nausea, vomiting and

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

Identification: : Ethanolamine UNNA: 2491 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Ethanolamine Illinois toxic substances disclosure to employee act: Ethanolamine Rhode Island RTK hazardous substances: Ethanolamine Pennsylvania RTK: Ethanolamine Minnesota: Ethanolamine Massachusetts RTK: Ethanolamine Massachusetts spill list: Ethanolamine New Jersey: Ethanolamine TSCA 8(b) inventory: Ethanolamine

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). CLASS E: Corrosive liquid.

DSCL (EEC):
R20- Harmful by inhalation. R36/37/38- Irritating to eyes, respiratory system and skin. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S28- After contact with skin, wash immediately with plenty of water. S36/37/39- Wear suitable protective clothing, gloves and eye/face protection. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 2

Reactivity: 0

Personal Protection: H

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 2

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
-SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II.

Other Special Considerations: Not available.

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Last Updated: 05/21/2013 12:00 PM

Health	3
Fire	0
Reactivity	0
Personal Protection	

Material Safety Data Sheet
Phosphoric acid, 85% MSDS

Section 1: Chemical Product and Company Identification

Product Name: Phosphoric acid, 85%

Catalog Codes: SLP5569, SLP4555, SLP1732

CAS#: Mixture.

RTECS: Not applicable.

TSCA: TSCA 8(b) inventory: Phosphoric Acid; Water

CI#: Not available.

Synonym: Phosphoric Acid 85%; Phosphoric Acid; Orthophosphoric acid

Chemical Name: Not applicable.

Chemical Formula: Not applicable.

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Phosphoric Acid	7664-38-2	85-88
Water	7732-18-5	12-15

Toxicological Data on Ingredients: Phosphoric Acid: ORAL (LD50): Acute: 1530 mg/kg [Rat]. DERMAL (LD50): Acute: 2740 mg/kg [Rabbit]. DUST (LC50): Acute: >850 mg/m 1 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, . Hazardous in case of skin contact (corrosive, permeator), of eye contact (corrosive). Slightly hazardous in case of inhalation (lung sensitizer). Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth and respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation of respiratory tract, characterized by coughing, choking, or shortness of breath. Severe over-exposure can result in death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, liver, skin, eyes, bone marrow. Repeated

or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged contact with spray mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged exposure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection. Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: of metals

Explosion Hazards in Presence of Various Substances: Non-explosive in presence of open flames and sparks, of shocks.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
Reacts with metals to liberate flammable hydrogen gas. Formation of flammable gases with aldehydes, cyanides, mercaptins, and sulfides.

Special Remarks on Explosion Hazards: Mixtures with nitromethane are explosive. (Phosphoric Acid)

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container. If necessary: Neutralize the residue with a dilute solution of sodium carbonate.

Large Spill:
Corrosive liquid. Poisonous liquid. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use water spray curtain to divert vapor drift. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of sodium carbonate. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Do not ingest. Do not breathe gas/fumes/ vapor/spray. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, combustible materials, metals, alkalis. May corrode metallic surfaces. Store in a metallic or coated fiberboard drum using a strong polyethylene inner package.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Face shield. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Boots.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
Phosphoric Acid TWA: 1 STEL: 3 (mg/m3) from ACGIH (TLV) [United States] TWA: 1 STEL: 3 (mg/m3) from OSHA (PEL) [United States] TWA: 1 STEL: 3 (mg/m3) from NIOSH TWA: 1 STEL: 3 (mg/m3) [Mexico]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Syrupy liquid Viscous liquid.)

Odor: Odorless.

Taste: Acid.

Molecular Weight: Not applicable.

Color: Clear Colorless.

pH (1% soln/water): Acidic.

Boiling Point: 158°C (316.4°F)

Melting Point: 21°C (69.8°F)

Critical Temperature: Not available.

Specific Gravity: 1.685 @ 25 C (Water = 1)

Vapor Pressure: 0.3 kPa (@ 20°C)

Vapor Density: 3.4 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:
Easily soluble in hot water. Soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Incompatible materials

Incompatibility with various substances: Reactive with oxidizing agents, combustible materials, metals, alkalis.

Corrosivity:
Extremely corrosive in presence of copper, of stainless steel(304), of stainless steel(316). Highly corrosive in presence of aluminum. Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Reacts with metals to liberate flammable hydrogen gas. Incompatible with sodium tetrahydroborate producing a violent exothermic reaction. Heat generated with: alcohols, glycols, aldehydes, amides, amines, azo-compounds, carbamates, caustics, esters, ketones, phenols and cresols, organophosphates, epoxides, combustible materials, unsaturated halides, organic peroxides. Formation of flammable gases, with aldehydes, cyanides, mercaptins, and sulfides. Formation of toxic fumes with cyanides, fluorides, halogenated organics, sulfides, and organic peroxides. Do not mix with solutions containing bleach or ammonia. Incompatible with nitromethane, chlorides + staiinless steel. (Phosphoric Acid)

Special Remarks on Corrosivity:
Minor corrosive effect on bronze. Severe corrosive effect on brass. Corrosive to ferrous metals and alloys.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 1530 mg/kg [Rat]. Acute dermal toxicity (LD50): 2740 mg/kg [Rabbit].

Chronic Effects on Humans: May cause damage to the following organs: blood, liver, skin, eyes, bone marrow.

Other Toxic Effects on Humans:
Extremely hazardous in case of inhalation (lung corrosive). Very hazardous in case of skin contact (irritant), of ingestion, . Hazardous in case of skin contact (corrosive, permeator), of eye contact (corrosive).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: Skin: Corrosive and causes severe skin irritation and can cause severe skin burns. May affect behavior (somnolence or excitement) if absorbed through skin. Eyes: Corrosive. Liquid or vapor causes severe eye irritation and can cause severe eye burns leading to permanent corneal damage or chemical conjunctivitis. Ingestion: May be harmful if swallowed. Causes irritation and burns of the gastrointestinal (digestive) tract. Causes severe pain, nausea, vomiting, diarrhea hematemesis, gastrointestinal hemmorrhaging, and shock. May cause corrosion and permanent tissue destruction of the esophagus and digestive tract. May affect behavior and urinary system, liver (hepatocellular damage, hepatic enzymes increased), blood (blood dyscrasia). May also

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

Identification: : Phosphoric acid (Phosphoric Acid) UNNA: 1805 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: Phosphoric Acid Illinois toxic substances disclosure to employee act: Phosphoric acid Illinois chemical safety act: Phosphoric acid New York release reporting list: Phosphoric acid Rhode Island RTK hazardous substances: Phosphoric acid Pennsylvania RTK: Phosphoric acid Minnesota: Phosphoric acid Massachusetts RTK: Phosphoric acid Massachusetts spill list: Phosphoric acid New Jersey: Phosphoric acid New Jersey spill list: Phosphoric acid Louisiana spill reporting: Phosphoric acid California Director's list of hazardous substances: Phosphoric acid TSCA 8(b) inventory: Phosphoric Acid; Water SARA 313 toxic chemical notification and release reporting: Phosphoric acid CERCLA: Hazardous substances.: Phosphoric acid: 5000 lbs. (2268 kg)

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada): CLASS E: Corrosive liquid.

DSCL (EEC):
R34- Causes burns. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S45- In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 0

Reactivity: 0

Personal Protection:

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Face shield.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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Last Updated: 05/21/2013 12:00 PM

SAFETY DATA SHEET

Version 3.5
Revision Date 04/02/2014
Print Date 04/15/2014

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name	:	Sulfolane
Product Number	:	88965
Brand	:	Fluka
Index-No.	:	016-031-00-8
REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	:	126-33-0

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

Identified uses : Laboratory chemicals, Manufacture 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 # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, Oral (Category 4), H302

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: Warning

Hazard statement(s)

H302	Harmful if swallowed.

Precautionary statement(s)

P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.
P330	Rinse mouth.
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	:	Tetrahydrothiophene 1,1-dioxide Tetramethylene sulfone
Formula	:	$C_4H_8O_2S$
Molecular Weight	:	120.17 g/mol
CAS-No.	:	126-33-0
EC-No.	:	204-783-1
Index-No.	:	016-031-00-8

Hazardous components

Component	Classification	Concentration
Sulpholane		
	Acute Tox. 4; H302	-

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
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
Carbon oxides, Sulphur oxides

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed.
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.

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

Contains no substances with occupational exposure limit values.

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

Safety glasses with side-shields conforming to EN166 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: Chloroprene
Minimum layer thickness: 0.6 mm
Break through time: 480 min
Material tested:Camapren® (KCL 722 / Aldrich Z677493, Size M)

Splash contact
Material: Nature latex/chloroprene
Minimum layer thickness: 0.6 mm
Break through time: 60 min
Material tested:Lapren® (KCL 706 / Aldrich Z677558, 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
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: crystalline 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: 20 - 26 °C (68 - 79 °F) - lit.
f)	Initial boiling point and boiling range	104 °C (219 °F) at 0.3 hPa (0.2 mmHg) - lit. 285 °C (545 °F) - lit.
g)	Flash point	177 °C (351 °F) - closed cup
h)	Evapouration rate	no data available
i)	Flammability (solid, gas)	no data available
j)	Upper/lower flammability or explosive limits	no data available
k)	Vapour pressure	no data available
l)	Vapour density	no data available
m)	Relative density	1.261 g/mL at 25 °C (77 °F)
n)	Water solubility	no data available
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
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
no data available

10.4 Conditions to avoid
no data available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
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 - mouse - 1,900 mg/kg

Inhalation: no data available

LD50 Dermal - rat - > 3,800 mg/kg

no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
Eyes - rabbit
Result: Mild eye irritation

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.

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

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
no data available

Additional Information
RTECS: XN0700000

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	LC50 - Carassius auratus (goldfish) - 140 mg/l - 24 h

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
Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

SARA 313 Components
SARA 313: 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, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Sulpholane	126-33-0	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date

Sulpholane	126-33-0	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Sulpholane	126-33-0	1993-04-24

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
H302	Harmful if swallowed.

HMIS Rating

Health hazard:	1
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	0
Fire Hazard:	1
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
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