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Production of Propylene Oxide from Propylene Using Patented Silver Based Catalyst

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Dear Dr. Seider and Professor Fabiano,

Enclosed you will find the solution to the design problem presented by Bruce M. Vrana, DuPont. The proposed process design is for the industrial production of propylene oxide from propylene. The oxidation catalyst, silver oxide (Ag₂O) supported on tungsten trioxide oxide (WO₃), oxidizes propylene to PO in high yield. The product is purified through adsorption-desorption cycle with monoethanolamine (MEA), and other byproducts are separated by distillation. The PO product is 99.9822% pure by mass and fits the purity specifications of industry leaders. The reactor effluent is fed through an adsorption-desorption cycle to remove the CO₂. The product from the cycle is then taken through two distillation towers which remove any unwanted side products. The proposed plant will be located on the U.S. Gulf Coast and has the capacity to produce 200MM lb/year of propylene oxide.

This report contains detailed process design, economic analysis, and conclusions and recommendations for the implementation of the plant. The proposed plant is found to be economically feasible. Except for the most extreme variations of the price of PO, variable costs, fixed costs, and total permanent investment, the IRR remains strongly positive indicating the high chance of this project’s success even if factors outside of the group’s control negatively affect its economics. It has an estimated IRR of 81.91% with a total NPV of $ 262,808,900. Most of the continuous operations in this process were modeled using Aspen Plus v8.6. Cost estimates for the equipment were obtained using the equations contained in *Process Design Principles, 3rd Edition*, by Seider, Seader, Lewin and Widagdo.

Thank you for the assistance afforded to us during this project.

Sincerely,

______________________________
Eric Schultz

______________________________
Mitchell Schwartz

______________________________
Kyle Yu
Production of Propylene Oxide from Propylene

Senior Design Project, CBE 459

Project submitted to: Dr. Warren Seider
Prof. Leonard Fabiano
Dr. Robert Riggleman

Project proposed by: Bruce M. Vrana, DuPont

Dept. of Chemical and Biomolecular Engineering
School of Engineering and Applied Science
University of Pennsylvania
April 5, 2016
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1.0 ABSTRACT

Propylene oxide (PO) is an important intermediate in the manufacture of propylene glycol (PG), polyether polyols and many other products. Conventional production of propylene oxide has many drawbacks. The most common method, the chlorohydrin process, produces chlorinated byproducts, which must be disposed of. Other processes produce a co-product, like styrene, which adversely affects production economics. A team of scientists at the Council of Scientific and Industrial Research (CSIR) in New Delhi has recently applied for a patent for a catalyst that oxidizes propylene to PO in high yield. The primary motivation behind this project was the production of PO without the unwanted side products of traditional methods by using the direct oxidation in CSIR’s patent.

Our proposed plant design produces 200 million lbs/year of propylene oxide from propylene and will be located on the U.S. Gulf Coast. Our plant is divided into four sections, namely feed material pretreatment, direct oxidation reaction, initial separation, and final distillation. The byproducts include carbon dioxide, acetaldehyde, acrylic acid, and acrolein. Carbon dioxide is separated through adsorption-desorption cycle with monoethanolamine (MEA), other byproducts are separated by distillation, and PO product is 99.9822% pure by mass. The cost of purchase of propylene is $1,100/tonne and the selling cost of PO is $2500/tonne. The process has an estimated IRR of 81.91% and an NPV of $262,808,900. This report provides a detailed design and economic analysis for PO production in the Gulf Coast. Process flow sheets, energy and utility requirements and reactor design have been considered during our analysis below. The total cost of equipment is $35,715,726. Except for the most extreme variations of the price of PO, variable costs, fixed costs, and total permanent investment, the IRR remains strongly positive indicating the high chance of this project’s success even if factors outside of the group’s control negatively affect its economics. Due to its low risk and high reward, a license for the catalyst described in the patent should be acquired, and this process should be developed.
2.0 INTRODUCTION

Propylene Oxide (CH₃CHCH₂O) is a colorless volatile liquid that is produced on a large scale industrially.²² Propylene Oxide (PO) is primarily used as an intermediate in the manufacture of propylene glycol (C₃H₆O₂), polyether pylyols and other products. Propylene glycol, PG, is used to make unsaturated polyester resins, environmentally-friendly antifreeze, cosmetics etc. PG can also be used as a humectant, solvent and preservative in food or tobacco products. Polyether polyol is an alcohol containing multiple hydroxyl groups. Polyether polyol is used for the production of polyurethane plastics, which have a wide range of applications including manufacture of: insulation, durable wheels and tires, high performance adhesives, hard plastics and hoses.

Conventional industrial production of PO has many drawbacks. Two general approaches are taken for PO production including the hydrochlorination route and the co-oxidation of propylene.¹¹ The traditional hydrochlorination route converts propylene to chloropropanols which are then dehydrochlorinated to create PO. The chlorinated byproducts of this process, both organic and inorganic salts, must be disposed of. The co-oxidation of propylene produces coproducts t-butyl alcohol and styrene, which can decrease the economic benefit of producing PO. As a result of these drawbacks, there has been extensive industry research on direct oxidation of propylene to make PO with high selectivity for reduced byproduct production.

The focus of this report is to make propylene oxide from propylene via direct oxidation to match the demand. The direct oxidation reaction is C₃H₆ (Propylene) + ½ O₂ = C₃H₆O (Propylene Oxide).¹⁰ The reactor feed streams are 95% pure (chemical grade) propylene available on plant site and 99.6% pure oxygen. The reference patent from the Council of Scientific and Industrial Research (CSIR) gives a laboratory selectivity of 100%.⁸ For industrial application, we assumed a 99.9% selectivity with other compounds being created including CO₂, acetaldehyde, acrylic acid, and acrolein. However, to make this process highly selective and produce propylene oxide at 99.9% selectivity a newly patented catalyst is used. There is no such catalyst used for industrial scale production today. A team of scientists from the Council of Scientific and Industrial research (CSIR) have applied for a patent for a catalyst (silver oxide [Ag₂O] supported on tungsten trioxide oxide [WO₃]).⁸ The laboratory research of CSIR for the catalyst is used as the basis of the design project.

The direct oxidation of propylene is a very exothermic reaction, and the reactor is cooled down by running boiler feed water through the shell side of the shell and tube reactor to produce steam. Once propylene oxide is produced, the main byproduct (CO₂) needs to be separated through adsorption. Monoethanolamine (MEA) is used as a solvent. Propylene oxide needs to be separated from acetaldehyde, acrylic acid, and acrolein. The purity of the final product is under the purity requirements of industry leaders and can be distributed to the entire PO market.
The proposed plant will be located in the U.S. Gulf Coast and will produce 200 million pounds per year of PO. This location was chosen due to its proximity to the propylene source plant. In the report below, multiple factors such as utility requirements, plant design and equipment costs are considered and discussed.
2.1 OBJECTIVE TIME CHART

Name: Production of Propylene Oxide from Propylene

Champions: Mr. Leonard Fabiano, Dr. Rob Riggleman, and Mr. Bruce M. Vrana

Project Leaders: Eric Schultz, Mitchell Schwartz, Kyle Yu

Specific Goals: Develop a direct oxidation of propylene to propylene oxide plant with a capacity of 200 MM lb/yr.

Project Scope: In Scope

Annual production of 200 million pounds of propylene oxide
Propylene oxide purity to industry standards
Market and Profitibility Analysis
Plant Design and Size
Reactor Design and Size

Out of Scope
Lab work to design and test catalyst for direct oxidation process
Process to produce catalyst
Distribution of final PO product
Process to produce chemical grade propylene
Design of catalyst packing

Deliverables: Mass and energy balances of the process
Equipment specifications, designs, and cost estimates
Detailed flow sheet diagrams and simulation results
Economic and profitability analysis, with an emphasis on overall feasibility
Reactor Design and Analysis

Time Line: Completed this design project within three months
3.0 TECHNOLOGY READINESS ASSESSMENT

3.1 INNOVATION MAP
3.2 BRIEF HISTORIES OF PREVIOUS TECHNOLOGIES

Propylene oxide has traditionally been produced using chlorohydrin processes. This process creates a large volume of chlorinated side products that are difficult to separate and then have to be sold as well. The high capital cost associated with the process eats heavily into the process.\textsuperscript{31}

Other processes have been created to avoid using chlorine including epoxidation reactions. However, this process produces 2.25 times more styrene than it does propylene oxide, which leads to greater economic volatility as the price of styrene fluctuates. Additionally, this process also has a high capital cost.\textsuperscript{31}

More recently, companies have aimed to develop processes that can produce propylene oxide while minimizing the amount of side products produced.\textsuperscript{31} Propylene can be reacted with hydrogen peroxide to produce propylene oxide and water. So far, no one has been able to develop and scale up a process to directly oxidize propylene, reducing both material and capital costs while making almost no side products.
3.3 PATENT DETAILS AND TECHNOLOGY IMPLEMENTATION

As mentioned in previous sections, there are many disadvantages to traditional methods of propylene oxide production. Propylene oxide processes are one of the few in modern industry that are still undergoing research and change. The chlorohydrin and co-oxidation processes are called “coproduct” processes and are difficult to deal with because of the necessary management or disposal of the two products. Direct oxidation of propylene with molecular oxygen is considered the “holy grail” of the PO industry and has been difficult to research and implement because allylic protons in the process were easily oxidized. Inventors Bal, Rajaram; Ghosh, Shilpi; Acharyya, Shankha Shubhra; Sarkar, Bipul; Pendem, Chandrashekar; Singha, Rajib Kumar from the Council of Scientific and Industrial Research (CSIR) in India have proposed a new catalyst system that helps direct oxidation of propylene to PO in high selectivity. American Chemical Society (ACS) Patent Watch group summarize the discovery, “The catalyst is based on silver supported on tungsten oxide nanorods (1:20 Ag/W ratio). Propylene conversions of 15.8–48.7% are reported at reaction temperatures of 200–400 ºC. PO selectivity is an amazing 100% at all temperatures except 400 ºC, where it drops to 97.1%.”

The catalyst from the CSIR patent is used for the primary reaction for our industrial sized propylene plant. The main objective of the patent is to “provide a process for preparation of Ag—W oxide catalyst for the selective conversion of propylene to propylene oxide with molecular oxygen.” The scope of our design fits in and does not overlap the main objective of the patent. The design uses the patent as a baseline. The 100% selectivity achieved by CSIR in the lab has been assumed to be 99.9% in the industrial scale process analyzed in this report. The production of the catalyst for use in the overall process is out of the scope of our design project. The design project assumes the catalyst can be imported from CSIR for a fixed price. However, a short summary of catalyst fabrication and general reaction procedure will be provided here for additional information.

<table>
<thead>
<tr>
<th>Step Number</th>
<th>Step Summary</th>
<th>Preparation Process Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Gel Preparation</td>
<td>Mixing AgNO₃, WO₃, H₂O, a surfactant cetyltrimethylammonium bromide (CTAB), a reducing agent hydrazine to obtain a gel</td>
</tr>
<tr>
<td>2</td>
<td>Gel Mixing</td>
<td>Mixing gel as obtained in step (1) with constant stirring for 2-6 h at room temperature ranging between 25-35° C.</td>
</tr>
<tr>
<td>3</td>
<td>Gel Filter, Wash and Dry</td>
<td>Filtering the gel as obtained in step (2) and washing with excess water and dried in an oven with temperature range of 100-120° C. For a period ranging between 6-18 h.</td>
</tr>
<tr>
<td>4</td>
<td>Calcining to Obtain Catalyst</td>
<td>Calcining the dried product as obtained in step (3) at temperature range of 300-750° C. for a period ranging between 4-10 h to obtain Ag—W oxide catalyst.</td>
</tr>
</tbody>
</table>
Using the patent information and data summaries, we designed an optimum process to make 200 MM lb/yr of PO from propylene. The focus of the design featured the process to make PO using the catalyst rather than the fabrication of the catalyst itself. The reaction takes place in a fixed bed down flow reactor which is run at 3 MPa and 350°C. Laboratory testing showed 100% selectivity of propylene to propylene oxide but industrially we are assuming the selectivity to be 99.9%. The weight hourly space velocity (WHSV) is 10,000 (g<sub>feed</sub>/hr)/g<sub>cat</sub> to obtain highest possible single pass conversion (36.3) and selectivity (99.9%).

The design team has based the designed process off of the patent but has not licensed the technology. The patent has been applied for, meaning that the research for the catalyst is finished. The technology is ready for implementation, following licensing for the design team and approval of the patent. As negotiations with CSIR can be sensitive, only public information resources for the catalyst are used for design, and no direct contact with CSIR has been made. Data from the patent is mainly obtained from lab tests and many assumptions for scale up to industry size process have been made for the process.

### 3.3.1 CATALYST TECHNICAL BACKGROUND

**Direct Oxidation of Propylene Possible Reactions**

<table>
<thead>
<tr>
<th>Product</th>
<th>Reaction</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(C_3H_6 + \frac{1}{2}O_2 \rightarrow C_3H_6O) (Propylene Oxide)</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(2C_3H_6 + 9O_2 \rightarrow 6CO_2 + 6H_2O) (Carbon Dioxide)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>(2C_3H_6 + \frac{3}{2}O_2 \rightarrow 3CH_3CHO) (Acetaldehyde)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>(C_3H_6 + O_2 \rightarrow C_3H_4O + H_2O) (Acrolein)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>(C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O) (Acrylic Acid)</td>
<td></td>
</tr>
</tbody>
</table>

### Table 3.2. Optimal Reaction Conditions (from Patent)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>350°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>3 MPa</td>
</tr>
<tr>
<td>WHSV</td>
<td>10,000 (mL&lt;sub&gt;feed&lt;/sub&gt;/hour)/g&lt;sub&gt;cat&lt;/sub&gt;</td>
</tr>
<tr>
<td>Catalyst Life Span (for regen)</td>
<td>30 hr</td>
</tr>
</tbody>
</table>

At the above conditions, the patent claims the catalyst has 100% selectivity, which would mean that there are no side products. However, at other conditions, CO2, water, and acetaldehyde are produced in small quantities. Additionally, other oxygenated products may exist in smaller quantities such as
acrolein and acrylic acid. The direct oxidation of ethylene to ethylene oxide (E to EO) process is a similar reaction and overall process to our P to PO process and has been used as a common baseline for assumptions for our process. Many of our process assumptions to fill in holes in the patent’s information base have been taken, by recommendation from professors and consultants, from the E to EO process that has been tested extensively from industrial applications. Assumptions of the catalyzed direct oxidation reaction from P to PO that our design group has made includes 99.9% selectivity of reacted propylene goes to the primary product reaction and 0.1% selectivity of reacted propylene goes to the side product reactions. Of the 0.1% reaction that goes to side products, 88% of unconverted propylene goes to production of CO₂ and water, 4% of unconverted propylene goes to production of acetaldehyde, 4% to acrylic acid, and 4% to acrolein. The ratio of side product production was not specified in the catalyst patent and was based off of the ethylene oxide industrial process.

From information gathered on the patent, the catalyst direct oxidation reaction is greatly exothermic. The energy released by the exothermic reaction is 23,053,000 kJ/hr or 6,400 kJ/s. The calculations of this are based on heat of formations of the reactants and products involved in the reaction along with the constant pressure specific heats of each one of the species. The amount of heat released from the reaction is huge and the adiabatic temperature rise of the reactor without a cooling system would be from 623 K to 4140 K. A dependable cooling system for the reactor is needed because selectivity and performance of the catalyst for the oxidation reaction decreases above 400°C. A shell and tube reactor is used in the process in order to capture excess heat from the reaction and to keep the reaction at a steady optimum temperature. The reaction occurs in the tube side of the reactor and boiler feed water is fed through the shell side in a suppressed vaporization process to remove excess heat.

From patent information, the catalyst life span before needing regeneration is about 30 hours. The catalyst deactivation time is about 30 hours because the reaction process produces carbon, or coke, which remains on the catalyst particle, reducing its effectiveness over time. Detail on the patent provides the assumption that the catalyst operates at 100% efficiency throughout its entire life span. Catalyst regeneration will be discussed in detail in later sections, but a summary of the design and reasoning is provided here. On site or in reactor regeneration is needed because of the short deactivation time. In reactor regeneration is not recommended because burning coke off at 500°C in reactor would create fumes that need to be vented and steaming the catalyst to strip off impurities would be difficult in the reactor. Fluidized Catalytic Cracking Unit (FCCU) will be used to continuously route deactivated catalyst into the regeneration unit. The optimal design agreed upon by the design group was two reactors in parallel with one regenerating while one is operating. The reactors would be switched every day (24 hours). This was decided upon to regulate the schedule of the reactor switching between regeneration and operation. Also, 24 hours gives a significant buffer under the catalyst deactivation time of 30 hours and
should ensure 100% efficiency of the catalyst over the 24 hours. In order to maintain a correct scope of the project, the assumption that the catalyst would operate at 100% of the patent’s specified efficiency through multiple regeneration and operation cycles was made.

The main advantages of the catalyst invention by CSIR are outlined in the patent.⁸ According to the scientists at CSIR, the main advantage is that the process converts propylene directly to propylene oxide without the need for additional catalyst or additional process steps. The process also provides a good conversion and very good selectivity to propylene oxide. This process uses pure oxygen instead of air. The process also does not produce too many side products, which is a major advantage, simplifying the process. The process also does not need additional reagents other than molecular oxygen and propylene in order to activate the reaction process. The catalyst is used in small amounts. The catalyst does not exhibit any signs of deactivation until 30 hours into contact with the reaction stream.
3.4 MARKET ANALYSIS

3.4.1 INDUSTRIAL USES OF PROPYLENE OXIDE

Most commonly, propylene oxide is used as an intermediate in the production of polyurethane. Polyurethane can be used to make both flexible and rigid foams. Flexible foams are used in items like household furniture and car seats. Rigid foams are used primarily for insulation in buildings.32

Additionally, propylene oxide can be used to make monopropylene glycol (MPG). MPG can be used to build housing panels, pipes, tanks and in coolants and antifreeze.32

In the coming years, there is an expected increase in polyeurathane demand across many different market segments, including the automotive industry and construction. Much of this will come from rising infrastructure spending in countries such as China, Brazil, Saudi Arabia, and Qatar. As these and other countries industrialize, they have rapidly rising disposable income, and rising infrastructure spending will follow. Traditionally, Europe has been dominant in the propylene oxide market, but the market share is expected to shift to North America and the Asia-Pacific region due to technological advances and rapidly growing economies in those regions.25

One restricting factor in the growth of the propylene oxide market is fluctuating raw material prices.25 This makes the process designed in this report especially competitive. The high selectivity of the catalyst and recycle stream for unreacted propylene create a high yield of propylene oxide, reducing the amount of raw materials that need to be purchased, and thus, the process’s dependence on fluctuating raw material prices.

The market for propylene oxide is highly competitive with major chemical companies including Dow, LyondellBasell, and BASF serving as major players.25 Normally, it is not advisable to enter such a well-established and fortified market, but this process provides a unique advantage over the competitors and thus, the ability to take away market share from the current industry leaders.

3.4.2 SIDE PRODUCTS

As the reaction proceeds with 99.9% selectivity, only small quantities of side products are produced. The side products from the reaction are carbon dioxide, water, acrylic acid, acetaldehyde, and acrolein. The group will dispose of the side products rather than try to sell them.

One issue is that the process gets rid of acrolein, water, and acrylic acid together in the second distillation column. In order to sell these products, two additional columns would have to be built to separate the three chemicals. Additionally, the amount of acetaldehyde produced is so small that it goes out with the propylene oxide, so an additional column would need to be built there as well to remove the traces of acetaldehyde. Storage would also have to be built to store the side products.
Still, there is one economical byproduct of the reaction. The direct oxidation of propylene to propylene oxide is highly exothermic. To keep the reactor at 350 degrees Celsius, steam is created. This steam is then used to heat both reboilers. The reactor generates 110,400 lb/hr of 150 lb steam, and the reboilers only use 22,100 lbs/hr, leaving over an extra 88,300 lbs/hr of steam. Steam sells for $0.007 per pound while boiler feed water only costs $0.002 per gallon or $0.00024 per pound. Thus, for every pound of propylene oxide produced, an additional $0.023 can be made from the extra steam, increasing sales by 2.04%.
3.5 CUSTOMER REQUIREMENTS

Propylene oxide is an important intermediate used for manufacture in industry of propylene glycol, polyether polyols and other products. PO is among the top 50 chemicals produced in the world by volume, and has an annual production rate of about 5 million tons.\(^2\) Traditional methods of PO production, as mentioned before, have many byproducts that are separated out after reaction, so the industry standards for PO product are quite specific. In order to maximize potential economic profit and minimize distribution problems, the process design accounted for the entire propylene oxide market.

3.5.1 INDUSTRY PROPYLENE OXIDE PURITY SPECIFICATIONS

The design group accounted for the entire PO market by ensuring that the PO product that is produced in the process was under the purity specs for all four industry leaders in propylene oxide purchases. The four companies that lead the purchase market for propylene oxide include Lyondell Bassell, Huntsman, Thyssenkrupp, and Petrorabigh.\(^2^9\)

| Table 3.3. Propylene Oxide Purity Requirements of Industry Leaders\(^2^9\) |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| Acidity (weight %)              | Lyondell Bassell| Huntsman        | Thyssenkrupp    | Petrorabigh     |
| **NS**                          | 0.005           | **NS**          | 0.005           | 0.002           |
| Aldehyde (weight %)             | 0.01            | 0.01            | 0.005           | 0.005           |
| Water (weight %)                | 0.02            | 0.025           | 0.01            | 0.01            |
| Total Impurities                | 0.02            | **NS**          | **NS**          | **NS**          |
| Assay                           | 99.98           | 99.9            | 99.97           | 99.9            |

**“not specified” in purity spec by company

To match the fitness-to-standard (FTS) customer requirements the product produced must conform to the customer’s specific purity requirements and will undergo purity checks, which compare the output and the specifications. The purity testing and distribution of the product are out of scope, but the product has been designed to satisfy all customer requirements. The side products produced in traditional PO production are separated from PO and sold on the market (providing a market for the side products exists). For the design in this report, the side products of CO\(_2\), acetaldehyde, acrylic acid, and acrolein have no significant economic gain associated with their sale.\(^2\) The amount of side products produced is too small to justify the infrastructure design and construction that is necessary to sell these products. Most of the side product created is CO\(_2\), which doesn’t have an economically feasible market around our plant’s location. CO\(_2\) production can also possibly create a carbon emission problem. However the process only produces around 180.22 ton/yr of CO\(_2\), which is very low for a plant of this size in industry. For comparison, in the city of Philadelphia, several emissions sources emit CO\(_2\) equivalent’s that
are magnitudes above the emission for our design. Temple University Campus emits CO₂ equivalent of 35,368 ton/yr, Trigen Energy Corporation emits CO₂ equivalent of 15,337 ton/yr and the Philadelphia Refinery emits CO₂ equivalent of 2,942,347 ton/yr. All of this data is from the United States Environmental Protection Agency. No CO₂ minimization, carbon sequestration or other further environmental measures relating to CO₂ are necessary. For changes in selectivity, a decrease in selectivity will lead to higher rates of CO₂ emissions. At 98.0% selectivity, an extreme situation, which is not regularly expected, the CO₂ emissions rate is 4063.9 ton/yr, which is still a low emissions rate.

Figure 3.1. Sensitivity Analysis of Reaction Selectivity on Carbon Dioxide Yearly Emissions
3.6 PRELIMINARY PROCESS SYNTHESIS.

As mentioned in the abstract and earlier sections, the primary motivation behind this project was to assess the economic viability of industrial sized direct oxidation of propylene oxide using Ag-W catalyst with high selectivity. The catalyst patent and the project problem statement were the main sources of initial information when starting the design process. Information on the catalyst patent was limited, as it had only been tested in lab and not on the industrial scale. The problem statement gave the scope of the project, as stated in the objective time chart, pricing information and plant location.

The data on the patent suggest propylene can be converted to propylene oxide through the direct oxidation of molecular oxygen reaction. Basic chemistry for the vapor phase reaction is:

\[
C_3H_6(\text{Propylene}) + \frac{1}{2}O_2 \rightarrow C_3H_6O(\text{Propylene Oxide})
\]

The reaction is very selective and the only product produced with the 100% selectivity found in the patent is propylene oxide. However, for the industrial scaled project, the design team has assumed 99.9% selectivity as mentioned in section 3.3 – Patent Details and Technology Implementation. The most important section of the plant is the direct oxidation reaction and the reaction conditions had to be chosen carefully, using information on the patent.

3.6.1 OPTIMIZATION OF REACTION CONDITIONS

To find ideal reaction conditions patent information regarding temperature, pressure, and silver loading was examined. The catalyst was inactive in the selective oxidation of propylene to PO at atmospheric pressure and temperatures below 150 °C. Choosing the correct temperature for the reaction depended on the effect of temperature on the selectivity and single pass conversion of the reaction. As temperature is increased from 200 – 400 ºC, the conversion of propylene increases (9% - 27%) but the selectivity decreases (91%-54%). The controlled variables for the temperature test were WHSV = 16000 hr⁻¹; pressure = 2 MPa; catalyst = 0.3 g; Ag:W weight ration 1:5 and time on stream = 6 hours.
The choice of pressure was similar to the choice of temperature, with a tradeoff of selectivity and conversion. The catalyst does not activate at atmospheric pressure. Raising the pressure from 1 MPa – 2 Mpa increases the selectivity (39% - 83%). Raising the pressure past 2 MPa to around 3 or 4 MPa, increases conversion but decreases selectivity (aprox. 83% - 55%). The control variables for the pressure tests were WHSV = 16000 hr\(^{-1}\); Temperature = 250 °C; catalyst = 0.3 g; Ag:W weight ratio in the catalyst = 1:5; Time = 6 h.

The choice of pressure was similar to the choice of temperature, with a tradeoff of selectivity and conversion. The catalyst does not activate at atmospheric pressure. Raising the pressure from 1 MPa – 2 Mpa increases the selectivity (39% - 83%). Raising the pressure past 2 MPa to around 3 or 4 MPa, increases conversion but decreases selectivity (aprox. 83% - 55%). The control variables for the pressure tests were WHSV = 16000 hr\(^{-1}\); Temperature = 250 °C; catalyst = 0.3 g; Ag:W weight ratio 1:5 and time on stream = 6 hours.\(^{38}\)
Increase in silver loading increased propylene conversion (15% - 26%) but decreased selectivity (83% - 58%) and also decreased the propylene oxide production rate. The controlled reaction conditions for the silver loading tests were WHSV = 16000 hr\(^{-1}\); Pressure = 2 MPa; Temperature = 250 °C; and time on stream = 6 hours.\(^{38}\)

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Loading of Ag (wt %)</th>
<th>Propylene Conversion (%)</th>
<th>Selectivity (%)</th>
<th>PO Production Rate (mol PO(_{cat})(^{-1})h(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Ag/WO(_3)</td>
<td>4.8</td>
<td>15.5</td>
<td>83</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>Ag/WO(_3)</td>
<td>8.3</td>
<td>21</td>
<td>67</td>
<td>13</td>
</tr>
<tr>
<td>3</td>
<td>Ag/WO(_3)</td>
<td>14.6</td>
<td>26</td>
<td>58</td>
<td>17</td>
</tr>
</tbody>
</table>

The optimal reaction conditions valued selectivity much more than the single pass conversion rate. The high selectivity of the catalyst towards PO was the main reason this patent was chosen. The conversion rate is single pass, and can be improved by adding a recycle stream. Adding a recycle stream loop can increase the overall conversion of propylene and save feedstock. The reaction conditions of temperature, pressure and silver loading were chosen based on the highest selectivity we could get. Initially, to maximize selectivity reaction conditions of: Ag:W-oxide weight ratio in the catalyst=1:20; Oxygen pressure: 3 Mpa; Temperature: 375° C; Reaction time: 6 h were chosen. The WHSV was tested at these conditions in order to maximize the propylene oxide selectivity. The results of the tests varying WHSV with all other reaction conditions constant helped find optimal WHSV.

<table>
<thead>
<tr>
<th>WHSV (ml feed/hr/g(_{cat}))</th>
<th>Propylene Conversion %</th>
<th>Propylene Oxide Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>49.1</td>
<td>44.9</td>
<td>91.4</td>
</tr>
<tr>
<td>6000</td>
<td>46.6</td>
<td>44.8</td>
<td>96.2</td>
</tr>
<tr>
<td>10,000</td>
<td>45.0</td>
<td>45</td>
<td>100</td>
</tr>
<tr>
<td>20,000</td>
<td>35.1</td>
<td>35.1</td>
<td>100</td>
</tr>
</tbody>
</table>

The final optimal reaction conditions, as chosen by this optimization method and analysis of each individual reaction condition as an independent variable is shown here. The reaction conditions were specified in section 3.6.1 – Catalyst Technical Background, but are reiterated here for clarity and reference.
Table 3.6. Optimal Reaction Conditions (from Patent)\textsuperscript{38}

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature:</td>
<td>350</td>
<td>Celsius</td>
</tr>
<tr>
<td>Pressure:</td>
<td>3</td>
<td>Megapascal</td>
</tr>
<tr>
<td>WHSV:</td>
<td>10,000</td>
<td>(gram$<em>{feed}$/hour)/gram$</em>{cat}$</td>
</tr>
<tr>
<td>Ag:W-Oxide wt ratio in catalyst:</td>
<td>1:20</td>
<td>Gram Ag to Gram W-oxide</td>
</tr>
<tr>
<td>Catalyst Life Span (for regen):</td>
<td>30</td>
<td>Hours</td>
</tr>
</tbody>
</table>

3.6.2 PRELIMINARY SEPARATIONS, UTILITIES, AND SAFETY

Generally, the separations section of the plant was designed to filter out the side products out the reactor effluent, so that the product propylene oxide stream was under all the industry standard purity specifications. Detailed information on separation processes is found in section 4.5 Initial Separation and section 4.6 Final Distillation. The side products CO$_2$, acetaldehyde, acrylic acid, and acrolein need to be separated out of a stream that contains, unreacted propylene, propylene oxide, excess oxygen, and inerts. Initially the carbon dioxide is separated out of the reactor effluent by an adsorption – desorption cycle. The stream is then split by a distillation tower between volatilities of propylene and acetaldehyde in order to recycle the propylene. The remaining side products are separated in a final distillation tower to hit the purity specification required. The propylene recycle stream was an economic decision to save on feedstock propylene operating cost versus the capital cost of building the recycle process. The distillation towers’ overhead condensers run with cooling water which require higher pressure to condense but save on operating cost of refrigerant.

Catalyst deactivation requires frequent regeneration.\textsuperscript{1} In order to not disturb continuous operation, two reactors were designed in parallel. One reactor will be operating while one reactor is undergoing regeneration. The high exothermic reaction in the reactor does not let the released heat go to waste. The heat of reaction is captured in the shell and tube reactor to convert boiler feed water to steam. This keeps the reactor at a stable temperature for optimal reaction conditions. The steam can then be used in the reboilers of the condenser tower. The reactor effluent is cooled down in a heat exchanger, which also heats up the feed before entering the reactor. The safety of the process will be discussed in detail in section 5.0 – Health and Safety Concerns.

The main safety concern in the plant is the possibility of combustion.\textsuperscript{26} Similar to related assumptions in the ethylene to ethylene oxide process, the dangerous range of propylene concentration for the process with pure oxygen is between 8.8 mol % and 36 mol % propylene.\textsuperscript{13} As long as the feed ratio is out of this flammability range, the risk of combustion is fairly low. The mixing point of oxygen and propylene can be a safety issue as a flammable combination of oxygen and propylene can exist while mixing. The mixing of oxygen and propylene is not done until the reactor; therefore, the reactor is the
biggest combustion hazard and should be designed and fitted with plenty of fireproofing equipment. This report focuses on optimizing a single design mostly aimed at the process reaction rather than the fireproofing aspect but we understand that further design considerations need to be taken into account when the reactors are actually built and installed.
3.7 ASSEMBLY OF DATABASE

Economic and process design decisions were fabricated based on information in the problem statement, market reports and University of Pennsylvania faculty and consultants expertise.

The baseline economic analysis originates from the parameters and guidelines in problem statement. The price for the product and feed were specified on the project recommendation, and were treated as the bottom line of which this design project was created. The prices of $2500/tonne for propylene oxide and $1100/tonne for propylene were specified. We made the assumption that the price of propylene oxide would be uniform across the market and was for propylene oxide that was produced to match industry standards. The chemical grade propylene at that price was assumed, from the problem statement, to be available as a coproduct at any amount at the plant site on the Gulf Coast. Our target propylene oxide production was specified as 200 million lb/year, therefore the propylene and oxygen feeds had to be adjusted to meet that mark. With this calculation the plant would yield approximately 2500 pounds propylene oxide per hour, 600,000 pounds propylene oxide per day and 200,000,000 pounds propylene oxide per year. The design actually predicts an additional 170,000 pounds of propylene oxide produced over the required 200 MM lb/yr. This additional production can act as additional profit as well as a buffer over the requirement.

Prices for different materials including catalyst, by products, utilities were found using information from parallel processes, consultant expertise, Dr. Seider’s profitability analysis lecture notes from CBE459, online databases and industry standards. The Ag-W catalyst was priced at $50/pound, which was estimated using information on ethylene to ethylene oxide reaction catalyst and consultant advice. Utilities of the process include 450 lb steam, 150 lb steam, 50 lb steam, cooling water, boiler feed water and electricity. The prices of utilities were obtained from profitability analysis lecture notes from CBE 459. The cost of utilities is as follows: $0.008 per lb of 450 pound steam, $.007 per lb of 150 pound steam, $0.006 per lb of 50 pound steam, $0.001 of cooling water, $0.052 per kWh of electricity, and $0.002 per gal of boiler feed water. Additionally, as mentioned in section 3.5.1 - Industry Propylene Oxide Purity Specifications, the only by product of the process that is viable to sell the excess 150 pound steam created by cooling the reactor. By product of 150 pound steam sold on the market is $0.007 per lb of 150 pound steam.

Aspen Process Economic Analyzer (APEA) was used for all equipment costing except for recycle pump, product storage tank, boiler feed water pump, and reactor. Costing spreadsheets were used for equipment costing not done by APEA. The reactor model was a shell and tube reactor to keep consistent temperature throughout the highly exothermic reaction process. The reactor sizing, design and costing was based on the similar reactor in the parallel process of E to EO. The process simulation and design was done using Aspen Plus. In order to model the thermodynamic and physical interactions between materials
in our process, the non-random two-liquid (NRTL) property method was used for the entire design. NRTL model calculates liquid activity coefficients for the simulation. NRTL was used for our non-ideal chemical system that had different vapor-liquid equilibrium, LLE and VLLE applications. The Aspen Physical Property System has many binary parameters build in for the NRTL property method. It is important to realize that Aspen approximates the parameters for the NRTL model to estimate the molecular interactions, so some differences may arise from the design and application.
4.0 PROCESS FLOW DIAGRAMS & MATERIAL BALANCES

4.1 OVERVIEW

The overall process is separated into four sections outlined and depicted in Figure 4.1 below. The five sections include:

1) Feed Material Pre-Treatment
2) Reactor Cycle
3) Steam Generation
4) Initial Separation
5) Final Distillation

![Figure 4.1. Overall Direct Oxidation to Propylene Oxide](image)

The following sections describe the five section process of making 200MM lbs/year of propylene oxide product from propylene through direct oxidation in the presence of a catalyst. A new patent has been applied for by the Council of Scientific and Industrial Research in New Delhi concerning the production of propylene oxide through catalyst based direct oxidation with very little to no side products. The process described in this section scale this catalyst technology from the laboratory to industrial proportion in order to determine the efficacy of large scale commercial continuous production of propylene oxide using this catalyst.

The process begins with the raw materials of the process, propylene and oxygen. As determined by the problem statement, chemical grade propylene is produced at the same plant site and is fed to the process by way of pipeline. For oxidation, the process will consume pure oxygen (99.6% pure) that is transferred to the process through a gulf coast pipeline at the desired pressure and temperature.

The oxygen feed and propylene feed are kept separate before the reactors. Before the reactor cycle, the oxygen feed is pre heated. As for the propylene feed, it is mixed with propylene recycle, pumped to high pressure, and preheated before it proceeds to the reactors. The reaction commences at
high pressure (30 bar) and high temperature (350°C) so the propylene feed needs to be pumped to the high pressure and both feeds need to be pre heated.

The two reactors are designed in parallel of each other in order for the process to regenerate the catalyst after sufficient reaction time. While one reactor is being used, the other reactor is regenerating the catalyst. The reaction is a direct oxidation of propylene with 99.6% pure oxygen, as opposed to air. Despite the 100% selectivity found in the laboratory, the process outlined below takes into account the high possibility that carbon dioxide and water will both be side products of the oxidation with a small amount of acetaldehyde, acrylic acid, and acrolein present. In addition to the propylene oxide product, steam is generated as a result of the largely exothermic reaction. The steam is used as utility throughout the plant and sold as a product.

After the reaction cycle, the reactor effluent enters an initial separation in the first stage distillation where the bulk of the propylene is separated from the bulk of the propylene oxide. The propylene is separated from the effluent mixture and recycled back to be fed back into the reactor as propylene feed. Then, the propylene oxide mixture moves from the bottom of the first stage distillation to the second stage distillation where it is further purified into the desired customer specified product.
Figure 4.2. Overall process flow diagram for the industrialization of propylene to propylene oxide through direct oxidation using a silver-based catalyst. Steam generation not depicted.
4.2 FEED MATERIAL PRE-TREATMENT

The beginning of the process deals with the pre-treating of the raw materials before they can be fed to the reactors for the reaction cycle. The propylene feed is distributed to our plant, from a co-producer on site, as chemical grade propylene. Chemical grade propylene has a minimum purity of 93-94% so our group assumed a purity of 95% for the propylene feed for our process. The impurities of propylene and oxygen are discussed in 4.5 Initial Distillation. The propylene is fed to our initial stage of pre-treatment at ambient temperature (25°C) as a liquid and at a pressure of 17 bar. The propylene has its first process encounter with a mixer where it is combined with the propylene mixture recycle stream coming from the initial separation. The recycle stream is 99.99% propylene in terms of mass and is at 17 bar. The feed propylene was chosen to be at ambient temperature to get rid of the need for refrigerants of any kind. Propylene is a liquid, at ambient temperature, at any pressure above 12 bar so the group chose a feed pressure of 17 bar to minimize the pumping necessary for the recycle pump, P-2, and the propylene feed pump, P-1.

In order to make 200MM lbs/yr of propylene oxide, the reactors would need to be fed 50,451.35 lb/hr of pure propylene, displayed in Table 4.1. Accounting for the purity of the propylene, the mixture of recycle and propylene would need to equal to 53,106.68 lb/hr of propylene. The material balance for the pre-treatment section of the process does not take into account the purity of the feeds so the oxygen and propylene feeds are assumed to be pure for the sake of mass balances. We will discuss the inerts in further sections. The material balance below in Table 4.1 shows the mass into the system equals the mass out of the system. Initially the propylene feed would have to be the total of 50,451.35 lb/hr but when the system reaches equilibrium the recycle will account for almost two thirds of the reaction propylene.
The propylene feed is assumed to be feed to the plant at ambient temperature and a storage vessel will hold the propylene at 17 bar in order to keep the propylene as a liquid. Beginning with the propylene as a liquid would make it easy for the process to pump the mixture up to the high pressure needed for the reaction. The reactor is going to be run at 30 bar so P-1 will pump the propylene mixture from 18 bar to 32 bar. The two extra bar will account for a 5 psi pressure drop due to friction in pipe (assumed by the group), a 15 psi pressure drop through the reactor (assumed), and a 2.72 psi pressure drop through the heat exchanger E-100. The total pressure drop throughout this initial process was calculated to be 1.57 bar.

**Table 4.1. Material Balance for Entire Pre-Treatment Section**

<table>
<thead>
<tr>
<th>COMPONENT</th>
<th>INLET</th>
<th>OUTLET</th>
<th>DIFFERENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PropFeed Recycle</td>
<td>OxyIn PropIn OxyIn</td>
<td></td>
</tr>
<tr>
<td>PROPY-01</td>
<td>18,340.6</td>
<td>32,111.56</td>
<td>50,452.16</td>
</tr>
<tr>
<td>ACROL-01</td>
<td>2.68E-07</td>
<td>2.68E-07</td>
<td>-1.8E-11</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>19.51021</td>
<td>19.51039</td>
<td>-0.00018</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>7039.736</td>
<td>7039.736</td>
<td>0</td>
</tr>
<tr>
<td>WATER</td>
<td>8.44E-12</td>
<td>8.44E-12</td>
<td>-2.1E-15</td>
</tr>
<tr>
<td>CARBO-01</td>
<td>12.63309</td>
<td>12.63296</td>
<td>0.00013</td>
</tr>
<tr>
<td>ACETA-01</td>
<td>2.24E-04</td>
<td>2.24E-04</td>
<td>-1.8E-08</td>
</tr>
<tr>
<td>ACRYL-01</td>
<td>1.31E-17</td>
<td>1.31E-17</td>
<td>-1E-21</td>
</tr>
<tr>
<td>Total Mass Flow (lb/hr)</td>
<td>18,340.6</td>
<td>32,143.7</td>
<td>7039.736</td>
</tr>
</tbody>
</table>

Pure oxygen, or in our case 99.6% pure oxygen is readily available in the Gulf Coast via pipeline. Pure oxygen for our process will be fed to the pre-treatment section at ambient temperature (25°C) and 32 bar. The reactor requires the feed at 30 bar but a 5 psi drop along the piping, 15 psi drop along the reactor, and a 0.53 psi drop through the exchanger E-200 requires 2 extra bar in the beginning of the process. The difference in pressure between the reactor and the feed will allow for the stream to move on its own without the need for pumping or compression.

**Table 4.2. Heat Exchanger Results**

<table>
<thead>
<tr>
<th>Stream</th>
<th>INLET</th>
<th>OUTLET</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Temperature (°C)</td>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>PumpedP</td>
<td>37.21</td>
<td>32</td>
</tr>
<tr>
<td>OxyFeed</td>
<td>25</td>
<td>32</td>
</tr>
<tr>
<td>RxnOut</td>
<td>350</td>
<td>30</td>
</tr>
</tbody>
</table>

After both streams have a high pressure, the streams need to be pre-heated before they can be loaded into the reactors. The temperature of the reactor was chosen to be 350°C, based on the patent
research described in the Section 6, so the heat exchangers E-100 and E-200 are responsible for getting the temperature of the feed streams up to 250°C. The heat exchangers were chosen to only increase the temperature to 250°C and not 350°C because of the highly exothermic behavior of the reactor. By feeding the oxygen and propylene into the reactor 100 degrees cooler than the reaction contents, the feed will act as a coolant to capture all of the heat generated by the oxidation reaction. The reactor effluent, at 350°C, is solely responsible for the heating of both the propylene and oxygen feeds using a counter-current shell and tube design. Table 4.2 above shows the exchanger input and output temperature and pressures.
4.3 REACTOR CYCLE

After the pressure is increased and the streams are heated, the feed streams move to the reactor cycle of the process. The reactor cycle is depicted below in Figure 4.4 with two reactors in parallel with each other.

![Figure 4.4. Process Flow Diagram for the Reactor Cycle](image)

The reactor cycle is composed of two packed bed shell and tube reactors in a parallel configuration. The catalyst is packed inside of the tubes while a cooling media is fed through the shell side. The direct oxidation reaction is highly exothermic and if held adiabatically would experience a temperature rise of over 3500 degrees. According to the patent, the reactor yielded the best results in the range of 150-400°C, 20-50 bar, and a WHSV (weight hourly space velocity) of 5,000-20,000 ml/hr/gm. In terms of selectivity of propylene oxide compared to side products, all temperatures below 400°C experienced a selectivity of 100% in the laboratory. However, the conversion of propylene significantly increased with temperature. Therefore, knowing that the reaction is very exothermic, 350°C was chosen to be the temperature the reactor would operate under in order to maximize selectivity and conversion and knowing we could heat our feed with our reactor outlet. At pressures higher than 20 bar, the conversion did not change. However, the selectivity decreased below 100% when the pressure exceeded 30 bar, producing our choice of 30 bar for the reactor operating pressure.
Shown in Table 4.3 is the material balance for the reactor cycle. Under the operating conditions chosen, the patent predicts that the process should be 100% selective and give 36.3% conversion of propylene to propylene oxide. However, the group decided that a 100% selective process in industry would not be an appropriate design decision. Therefore, the group determined a 99.90% selectivity would account for the production of side products. Of the 0.10% that did not go into producing propylene oxide, we also made assumptions as to which side products were made and how much of them were made. In the oxidation reaction to produce ethylene oxide, mostly water and carbon dioxide are the relevant side products. Without any sources giving reliable data on the selectivities within the side products we assumed that 88% of the unreacted propylene would go towards producing carbon dioxide and water. The final 12% of unreacted propylene is equally divided into producing acetaldehyde, acrolein, and acrylic acid, three of the side products mentioned throughout industrial oxidation research.

In order to make the desired 200MM lb/yr of propylene oxide, 25,252 lb/hr of propylene oxide must come out of the reactor effluent. Table 4.3 shows that 25,296.80 lb/hr of propylene oxide comes out of the reactor effluent which gives 44 lb/hr of leeway for distillation and separation. The reactor effluent is mostly composed of propylene (55.8% by mass) and propylene oxide (44.0% by mass) totaling 99.8% by mass of the mixture.

\[
\dot{V}_{\text{feed}} = 29,508.70 \, \text{ft}^3 ; \quad WHSV = 10,000 \, \frac{\text{mL/ hr}}{\text{g cat}}
\]

\[
\frac{\dot{V}_{\text{feed}}}{WHSV} = \text{mass cat} = 184.22 \, \text{lbs}
\]

Equation 4.1. Mass of catalyst needed for each reactor
The reactor cycle is set up in a parallel configuration in order for the plant operators to regenerate the catalyst after 24 hours of reacting. According to the patent, the catalyst does not deactivate until 30 hours so a 24-hour cycle time is an appropriate choice. The reactors will never be running at the same time. The calculation was done using Equation 4.1 to determine the amount of catalyst needed in each reactor based on a chosen 10,000 WHSV. Each reactor needs to contain 184.22 pounds of catalyst to give the desired 200MM lb/yr of propylene oxide. One advantage of using this new technology is the small amount of catalyst that is needed to achieve the high selectivities and conversions.
4.4 STEAM GENERATION

The reactor manages to produce 4,957,297 watts of energy which needs to be captured by a cooling media or the reactor would have a temperature increase of 3510°C. In order to keep the reactor at a constant 350°C, boiler feedwater is fed to the shell side of the operating reactor. The cycle is depicted in Figure 4.5 below.

![Figure 4.5. Steam generation cycle flow diagram](image)

The steam generation cycle utilizes a suppressed vaporization design. Boiler feedwater is necessary for the cooling media fed through the reactors because it is demineralized and will not cause fouling of the reactor tubes. Standard cooling water will cause fouling in the tubes of the reactor. The boiler feedwater is pumped up to high pressure at 12 bar and fed to the reactor. The heat released by the tubes due to the reaction is captured by the 110,361 lb/hr of boiler feedwater and increases the temperature of the water to approximately 181°C. 150lb steam has a pressure of 10.34 bar and 181°C. When the boiler feedwater exits the reactor at 12 bar and 181°C it is a saturated liquid stream. The exit water stream is sent to a flash drum, F-100, where the pressure is dropped to 10.34 bar which generates the 150lb steam. From the F-100 flash drum, 22,068 lb/hr of 150lb steam is sent to DST-100 and DST-200 while the remaining 88,293 lb/hr of 150lb steam is sold to the customer. The 150lb steam at 181°C allows for the proper greater than 10° driving force in the distillation tower reboilers.
4.5 INITIAL DISTILLATION

The initial distillation stage of the propylene oxide production process is broken in three different sections: carbon dioxide removal, distillation separation, and recycle. The initial distillation stage is depicted in the process flow diagram below in Figure 4.6.

![Process flow diagram of the initial distillation stage](image)

Figure 4.6. Process flow diagram of the initial distillation stage

After the reactor cycle and the reactor effluent has pre-heated the reactor feeds, the stream enters the carbon dioxide removal unit. The reaction is assumed to make a small amount of carbon dioxide relative to the propylene oxide but the carbon dioxide needs to be removed from the system to prevent buildup in the process units and piping. Possible solutions included a flash drum to vaporize the carbon dioxide, membrane separation, and solvent separation. The flash drum was the simplest of solutions but due to lack of component interaction property data in Aspen Plus, the group decided that a solvent separation apparatus would be ideal to remove the carbon dioxide from the process stream. The design for the carbon dioxide removal unit is based on the MEA-CO₂ adsorber proposed in Hammond et al. 2009. This adsorber is responsible for an 80% removal rate of the carbon dioxide in the CO₂Feed stream along with 100% oxygen, 5% water, and 0.00001% propylene removal. These removal rates of oxygen, water, and propylene were chosen based on industry consultant, professor, and Hammound et al. 2009 recommendations. The resulting CO₂Out stream will be discharged to the atmosphere. While this may be a carbon-emitting source, it only contributes less than 200 metric tons per year of CO₂ to the atmosphere. The small amount of carbon dioxide not removed by the adsorber would eventually come to an equilibrium in the system and has a chance to remove itself from the process via the DistVap1 stream off DST-100.
After most of the carbon dioxide has been removed from the process stream, the next objective is to separate out the propylene from the product mixture. The initial distillation tower, DST-100, has 23 stages and operates at a molar reflux ratio of 3.56, which is twenty percent above the minimum reflux ratio. The tower manages to achieve a split of 99.975% of propylene into the distillate and 99.923% of propylene oxide into the bottoms. The distillate stream runs through a partial condenser producing both vapor, DistVap1, and liquid, Recycle, distillate streams. A total of 32,111.56 lb/hr of propylene is recycled to the pre-treatment stage of the process while the process loses approximately 8.08 lb/hr of propylene to the product and waste streams. Of the propylene that enters the reactor, the process loses 0.016%. A pump, P-3, is needed to transfer the recycled propylene stream back to the propylene feed.

In order to maximize economic efficiency, the condenser, CD-1, was chosen to operate at a pressure of 17 bar in order for the condenser to utilize cooling water as the cooling media instead of an expensive refrigerant. The top stage temperature of the distillation tower is 40°C so cooling water at 30°C would bolster a more than enough temperature driving force for condensing.

The bottoms of the first distillation column moves on to the second stage distillation where the product is separated from water and acrylic acid. The bottoms from the first distillation yields 25,302.6 lb/hr with propylene oxide making up 99.9% of that mixture. The water and acidity contents are too high to meet propylene oxide customer demands, thus, the final distillation is needed for product purification.

**Impurities**

The oxygen used in the process is fed to the plant with 99.6% purity. Therefore, the process will cycle the impurities, most likely nitrogen, round in recycle and cause buildup of undesired waste. However, the initial distillation column is designed with both liquid and vapor distillates. The liquid

---

**Table 4.4.** Overall material balance on the initial distillation stage

<table>
<thead>
<tr>
<th>COMPONENT</th>
<th>INLET</th>
<th>OUTLET</th>
<th>DIFFERENCE</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CO2Feed</td>
<td>Recycle</td>
<td>Bottoms1</td>
<td>DistVap1</td>
</tr>
<tr>
<td>PROPY-01</td>
<td>32119.68</td>
<td>32111.56</td>
<td>1.66</td>
<td>6.42</td>
</tr>
<tr>
<td>ACROL-01</td>
<td>0.98</td>
<td>2.68E-07</td>
<td>0.98</td>
<td>3.44E-12</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>25296.80</td>
<td>19.51</td>
<td>25277.29</td>
<td>9.46E-04</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td>19.60</td>
<td>0.00E+00</td>
<td>19.60</td>
<td>0</td>
</tr>
<tr>
<td>WATER</td>
<td>21.33</td>
<td>8.44E-12</td>
<td>20.26</td>
<td>9.62E-18</td>
</tr>
<tr>
<td>CARBO-01</td>
<td>63.20</td>
<td>12.63</td>
<td>1.47E-06</td>
<td>6.66E-03</td>
</tr>
<tr>
<td>ACETA-01</td>
<td>1.15</td>
<td>2.24E-04</td>
<td>1.15</td>
<td>7.69E-09</td>
</tr>
<tr>
<td>ACRYL-01</td>
<td>1.25</td>
<td>1.31E-17</td>
<td>1.25</td>
<td>4.45E-24</td>
</tr>
<tr>
<td>Total Mass Flow (lb/hr)</td>
<td>57524.0</td>
<td>32143.7</td>
<td>25302.6</td>
<td>6.4</td>
</tr>
</tbody>
</table>
distillate is composed of the unreacted propylene that is recycled and the vapor distillate acts as a purge for the inerts and leftover carbon dioxide. The 0.4% of inerts in the oxygen stream will exit in the vapor distillate rather than buildup in the reactor cycle process equipment.
4.6 FINAL DISTILLATION

The final step in the process is the final distillation stage where the process stream is further separated into the liquid product stream and the waste stream.

![Figure 4.7. Overall mass balance of the final distillation stage](image)

The feed from the initial distillation contains water, acrylic acid, acetaldehyde, propylene, and mostly propylene oxide. However, the stream has too much water and acrylic acid to meet the customer specifications. To meet the desired specifications, a final separation must be made between the water, heavy key, and the acrolein, light key. The top stage of the tower is almost 35°C when it operates at atmospheric pressure, so assuming a 5 degree temperature driving force, the condenser can utilize cooling water as the cooling media to save on expenses.

<table>
<thead>
<tr>
<th>COMPONENT</th>
<th>INLET SepFeed2</th>
<th>OUTLET Product</th>
<th>DIFFERENCE</th>
<th>BOTTOMS2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PROPY-01</td>
<td>1.66</td>
<td>1.66</td>
<td>8.54E-15</td>
<td>0.00</td>
</tr>
<tr>
<td>ACROL-01</td>
<td>0.98</td>
<td>0.84</td>
<td>0.14</td>
<td>0.00</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>25277.29</td>
<td>25272.65</td>
<td>4.64</td>
<td>0.00</td>
</tr>
<tr>
<td>OXYGE-01</td>
<td></td>
<td></td>
<td></td>
<td>0.00</td>
</tr>
<tr>
<td>WATER</td>
<td>20.26</td>
<td>0.85</td>
<td>19.41</td>
<td>0.00</td>
</tr>
<tr>
<td>CARBO-01</td>
<td>1.47E-06</td>
<td>1.47E-06</td>
<td>3.24E-23</td>
<td>0.00</td>
</tr>
<tr>
<td>ACETA-01</td>
<td>1.15</td>
<td>1.15</td>
<td>1.88E-06</td>
<td>0.00</td>
</tr>
<tr>
<td>ACRYL-01</td>
<td>1.25</td>
<td>9.09E-12</td>
<td>1.25</td>
<td>0.00</td>
</tr>
<tr>
<td>Total Mass Flow (lb/hr)</td>
<td>25302.59</td>
<td>25277.15</td>
<td>25.44</td>
<td>0.00</td>
</tr>
</tbody>
</table>
The final product ends up with all of the propylene, all of the acetaldehyde, and most of the acrolein along with over 99.8% of the propylene oxide from the feed stream. 95.8% of the water was separated from the product stream and virtually 100% of the acrylic acid is removed via the Bottoms2 waste stream. The product stream finishes the separation 99.98% pure by mass with acrolein, acetaldehyde, water, and propylene as the majority of the undesired components. In the final distillation, 4.64 lb/hr, or 0.018%, of the propylene oxide is lost via the Bottoms2 waste stream. The final product stream flow rate of 25,277.15 lb/hr is approximately 25 lb/hr over the needed product mass flow to produce 200MM lb/yr of propylene oxide.
5.0 HEALTH AND SAFETY CONCERNS

5.1 FEED RATIO

The main safety concern for the direct oxidation of propylene to propylene oxide is the possibility of combustion. In the direct oxidation of ethylene, oxygen is fed with ethylene at a 10:1 mass ratio, which is an 8.77:1 molar ratio (10.2 mol % ethylene).\textsuperscript{13}

According to Linde, propylene is at risk of combustion when in volume (or molar) concentrations of between 2.0% and 10.5% in air. This process uses oxygen instead of air in the feed, altering the dangerous propylene concentration range. Thus, the dangerous range of propylene concentration for this process would fall between 8.8 mol % and 36 mol % propylene. This process uses a fuel-rich feed of 66.5 mol % propylene, well outside the dangerous range.

Additionally, the oxygen and propylene feeds are not mixed until entering the reactor, preventing them from entering in an unsafe ratio at the mixing point and possibly combusting.

Multiple redundant process controls will need to be placed to monitor the flow rates of oxygen and propylene into the reactor that can automatically shut down the plant if the flow rates begin to stray from the desired values, increasing the risk of explosion. There is an especially high risk of this during plant startup when the recycle stream has not come to equilibrium.

5.2 OTHER SAFETY CONCERNS

Employees will need protective gear when working on site. This will include flame retardant clothing, helmets, safety glasses, gloves, steel-toed boots, and earplugs. Smoking or any other activities with open flames or sparks will be banned on the premises to reduce the risk of igniting the oxygen. First aid and burn kits need to be available on site along with fire extinguishers for any small blaze to prevent it from igniting the oxygen. Safety training will be required of all employees and guests. Each employee must know how to use each piece of equipment safely and must know that if anything seems wrong, they need to shut down the plant.
6.0 REACTOR DESIGN

The direct oxidation reaction of propylene to propylene oxide over Ag-W-oxide catalyst is the main reaction in our process. The general outline of the reaction mechanism is described in figure 1 below.\textsuperscript{10}

![Figure 6.1. Mechanism for Formation of Propylene Oxide\textsuperscript{9}](image)

Initially, oxygen molecule dissociates over the metallic silver and the silver oxide (Ag\textsubscript{2}O) species with the silver to oxygen bond length of 2.349 angstroms is formed.\textsuperscript{10} The oxygen associated with the silver molecule enables creation of a cyclic transitions state, where the formation of the propylene double bond is followed by the insertion of an oxygen molecule into the double bond of propylene to form propylene oxide. The abstraction of the oxygen atom to the double bond of propylene to form propylene oxide is taking place according to the Langmuir-Hinshelwood mechanism.
To find whether the WO₃ base is the necessary and optimal for the P to PO reaction, several other catalyst bases were tested for catalytic activity. Table 6.1 shows the catalytic activity of the silver catalyst supported on different metal oxides. Performance of other metal oxides, when compared to tungsten oxide, was not up to par. The larger and irregular particles of entry 3 lead to bad propylene oxide selectivity, showing the importance of the nanorods that are prepared for the patented catalyst. Also silver and tungsten oxide alone, as in entries 1 and 2, do not exhibit any activity.

Table 6.1. Selectivity Analysis of Catalyst Base on Catalytic Activity

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Loading of Ag (%)</th>
<th>Propylene Conversion (%)</th>
<th>Selectivity (%)</th>
<th>PO Production Rate (mol PO₅cat⁻¹h⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Propylene Oxide</td>
<td>Acrolein</td>
</tr>
<tr>
<td>1</td>
<td>Ag</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>WO₃</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>Ag/WO₃</td>
<td>5</td>
<td>3</td>
<td>5</td>
<td>35</td>
</tr>
<tr>
<td>4</td>
<td>Ag/WO₃</td>
<td>4.8</td>
<td>15.5</td>
<td>83</td>
<td>8</td>
</tr>
<tr>
<td>5</td>
<td>Ag/Cr₂O₃</td>
<td>4.8</td>
<td>Negligible</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>Ag/MoO₃</td>
<td>4.8</td>
<td>5</td>
<td>49</td>
<td>29</td>
</tr>
<tr>
<td>7</td>
<td>Cu/WO₃</td>
<td>4.7</td>
<td>4</td>
<td>52</td>
<td>12</td>
</tr>
<tr>
<td>8</td>
<td>No Catalyst</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
6.1 REACTOR DESIGN ASSUMPTIONS

The direct oxidation reaction in the process is based on the information gathered from the patent. Incomplete data from the patent means the design team needed to make many assumptions in the reactor design. Side product selectivity was not specified in the patent, so assumptions about side products were made based on parallel process ethylene to ethylene oxide. In the E to EO process the main side product was CO₂ so we assumed 88% of side reactions are going to production of CO₂.¹³ The E to EO process also lead to the assumption of the side reactions of 4% going to production of acetaldehyde, 4% going to production of acrolein, and 4% going to production of acrylic acid. Table 6.2 shows that there are a range of temperatures where 100% propylene oxide selectivity exists over the patented catalyst. Therefore the assumption of same conversion, selectivity, and yield despite feed to reactor at 250°C instead of 350°C was made. The temperature of the reactor has been shown to be not sensitive to small changes, only sensitive to temperature going outside of a specified range. For the cooling system in the shell and tube reactor, we assumed 99% of heat from reactor to steam based on advice from consultants. The heat loss to environment from a shell and tube reactor where the reaction is occurring in the tubes, is minimal. The purity specifications for the product is the lowest in each category from four industry leading companies that purchase propylene oxide. The design group assumed that these four companies would give a good baseline for the product purity requirement for the entire market. Customer purity specs are discussed in detail in section 3.5.1 – *Industry Propylene Oxide Purity Specifications*. With the purity specs built into the design, the product should be of consistent quality and purity, which will satisfy the customer. With different streams traveling around the process, the assumption of only having reactions occur in the reactor was necessary for the design group to make. Reactions in material streams, pumps, pipes, towers etc. were considered out of scope for the design process. These reactions outside of the reactor, have less than optimal reaction conditions and also no catalyst. The reactions will be of minimum extent and would be too difficult to consider into the design process. Catalyst is assumed to be operating at full efficiency throughout the reaction cycle until regeneration and full efficiency even through multiple regenerations.¹ The catalyst patent did not specify, past the deactivation time, the actual drop in catalyst efficiency through multiple regeneration processes. Also for the time while the catalyst is on stream, Table 6.3 shows that from 1-24 hour time on stream, propylene conversion, propylene oxide yield and selectivity stay constant. The catalyst will be replaced if the efficiency goes down after multiple regenerations.
6.2 REACTOR DESIGN SYNTHESIS AND ALTERNATIVES

The reactor conditions are covered in section 3.6.1 – Optimization of Reaction Conditions. An overview is given in tables 6.2 – 6.5 for clarity and reference. The effects of conditions such as temperature, pressure, weight hourly space velocity (WHSV), and time on stream were studied to find optimum reaction conditions. Reaction conditions decided on were temperature of 350 Celsius, 3 megapascal, 10000 (ml feed/hour)/gramcat, Ag-W-oxide weight ratio of 1:20 grams silver per grams W-oxide, and 24 hours on stream before regeneration.

Table 6.2. Selectivity Analysis of Reactor Temperature on Propylene Conversion, Propylene Oxide Yield and Selectivity

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>15.8</td>
<td>15.8</td>
<td>100</td>
</tr>
<tr>
<td>250</td>
<td>20.3</td>
<td>20.3</td>
<td>100</td>
</tr>
<tr>
<td>300</td>
<td>24.6</td>
<td>24.6</td>
<td>100</td>
</tr>
<tr>
<td>350</td>
<td>36.3</td>
<td>36.3</td>
<td>100</td>
</tr>
<tr>
<td>400</td>
<td>48.7</td>
<td>47.3</td>
<td>97.1</td>
</tr>
</tbody>
</table>

Table 6.3. Selectivity Analysis of Time on Stream on Propylene Conversion, Propylene Oxide Yield and Selectivity

<table>
<thead>
<tr>
<th>Time on Stream (h)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>44.8</td>
<td>44.8</td>
<td>100</td>
</tr>
<tr>
<td>6</td>
<td>45.0</td>
<td>45.0</td>
<td>100</td>
</tr>
<tr>
<td>12</td>
<td>45.1</td>
<td>45.1</td>
<td>100</td>
</tr>
<tr>
<td>18</td>
<td>45.4</td>
<td>45.4</td>
<td>100</td>
</tr>
<tr>
<td>28</td>
<td>44.9</td>
<td>44.9</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 6.4. Selectivity Analysis of Oxygen Pressure on Propylene Conversion, Propylene Oxide Yield and Selectivity

<table>
<thead>
<tr>
<th>Reaction Pressure (MPa)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>17.3</td>
<td>17.3</td>
<td>100</td>
</tr>
<tr>
<td>3</td>
<td>45.0</td>
<td>45</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>46.1</td>
<td>43.8</td>
<td>95.1</td>
</tr>
<tr>
<td>5</td>
<td>47.3</td>
<td>39.9</td>
<td>84.3</td>
</tr>
</tbody>
</table>

Table 6.5. Selectivity Analysis of WHSV on Propylene Conversion, Propylene Oxide Yield and Selectivity

<table>
<thead>
<tr>
<th>WHSV (ml feed/h/gcat)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>49.1</td>
<td>44.9</td>
<td>91.4</td>
</tr>
<tr>
<td>6000</td>
<td>46.6</td>
<td>44.8</td>
<td>96.2</td>
</tr>
<tr>
<td>10000</td>
<td>45.0</td>
<td>45</td>
<td>100</td>
</tr>
<tr>
<td>20000</td>
<td>35.1</td>
<td>35.1</td>
<td>100</td>
</tr>
</tbody>
</table>
The shell and tube reactor for the direct oxidation of propylene over Ag-W-oxide catalyst was designed similar to a heat exchanger. The shell and tube reactor was chosen because of the largely exothermic reaction and a need to keep constant temperature. The reaction will occur in the tube side of the reactor and the shell side could flow boiler feed water for temperature control. The shell side is used for cooling the reactor, and without a cooling system, the reactor would heat up adiabatically to 4140 K. The shell side of the reactor uses the suppressed vaporization process to cool the reactor and create steam. Suppressed vaporization was chosen because heat transfer of liquid water in the shell would be more easily regulated than having vaporization occur on the shell side of the reactor. Heat transfer between the tube and the liquid on the shell side would also be better than heat transfer between the tube and gas on the shell side. The shell side of the reactor is discussed in further detail in section 6.4 – *Choice of Cooling Mechanism*.

The reactor design was split into two parts. The first part is the volume of the reactor tubes, which is related to the reaction of propylene to PO. The volume of the reactor is determined from weight hourly space velocity required from the patent specifications. The second part is the surface area of the reactor tubes which is related to the heat transfer of the shell and tube of the reactor. The surface area is determined from heat exchanger calculations based on heat released from the reaction. The ratio of the volume and surface area was then used to pick geometry for the tubes in the reactor. The tubes of the reactor contain the catalyst and flow the feedstock through.

To determine the necessary volume of the reactor tubes the WHSV of 10,000 (ml\textsubscript{feed}/hour)/gram\textsubscript{cat} given by the patent was used. The WHSV of the catalyst tells us the ratio of feed volumetric flow rate to grams of catalyst needed. Using the WHSV and the volumetric flow rate of feed the design team was able to find the reaction needed 184 pounds of catalyst. The void fraction of catalyst packing and catalyst density were not specified in the patent source or the problem statement so a 40% void fraction was assumed. The void fraction assumption comes from the average void fraction of similarly shaped particles, and this assumption was validated by consultants. The catalyst density was assumed to be similar to the catalyst density of the tungsten oxide support, which was 7.16 g/cm\textsuperscript{3}. Using the void fraction and density of catalyst, a volume of around 7000 cm\textsuperscript{3} or 0.007m\textsuperscript{3} was calculated.

To determine the necessary surface area of the tubes for proper heat transfer and cooling of the reactor, the heat of reaction calculation was done. Using ASPEN and doing heat of formation calculations by hand for the reaction, a figure of 6400 KJ/s was found for the heat released by the reaction. To find surface area of tubes needed for this heat to be exchanged, the log mean temperature difference and overall heat transfer coefficient was needed. The overall heat transfer coefficient was assumed to be 102.2 J/ M\textsuperscript{2}*s*K from table 18.5 in *Product and Process Design Principles* textbook. The log mean temperature
difference was calculated using adiabatic temperature rise of 623 K to 4140 K of the reactor. A surface area of around 49.7 m² was calculated for the tubes.

Using the method of volume and surface area to find geometry of the tubes for the reactor yielded 3 alternatives for the reactor design. The alternatives are small diameter tubes with 100% packing, larger tubes with catalyst packed in one section, and larger tubes with catalyst spread out throughout the tube. The first alternative of small tubes with 100% packing originates from the ratio of surface area to volume. With the necessary surface area (49.7 m²) being so much greater than the required volume (0.007 m³), the true ratio with 100% packing of the tubes would yield a diameter of 0.166 inches. This small diameter is a result of a small amount of catalyst being needed and a large amount of heat being generated. The drawbacks of these reactor is that the tubes are too small and too much pressure drop would be required to move the feed through the reactor. The second alternative of larger tubes with the catalyst packed in one section fixes the problem of high pressure drop in the reactor while also keeping 100% packing in the small section. The thought process behind this reactor was to keep 100% packing for full contact of catalyst and feedstock. However if the catalyst is all packed into one section, all the reaction would be occurring in that one section and all of the heat released would be in the section. This results in too much heat released in one spot along the tube’s length and cooling the reactor becomes an issue. The entire surface area of the tube would not be used for the heat exchange and the temperature would be unregulated. The last alternative design is the larger tubes with the catalyst spread out along the length of the tube. This alternative combines the previous two designs and has good volume for pressure drop as well as good surface area for heat exchange. The reaction is spread out which spreads out the heat released and thus cooling of the reactor on the shell side is more regulated. Also the volumetric flow rate of the feed is still in the ratio with the catalyst, which is specified by the WHSV. The drawback of this design is less contact time than 100% packing of catalyst in the first two designs. However, this was chosen as the best design by the group because of the good heat exchange and the reasonable pressure drop. The reaction was assumed to still be functional without 100% packing because the reactor was designed according to and adhering to the WHSV specified in the patent. The patent only specified WHSV and did not specify packing or contact time considerations.
6.3 SIMILARITIES WITH THE ETHYLENE OXIDE PROCESS

The direct oxidation of ethylene to ethylene oxide with a silver based catalyst was used as a general model for the design of this process with a few major changes. One change came in the ratio of the feeds. Ethylene and oxygen are mixed in a 1:10 mass ratio, which was impossible for this process as that ratio of propylene to oxygen would put it in the unsafe combustion range. Additionally, the propylene to propylene oxide process uses a fuel rich feed instead of an oxygen rich feed. This change was made because the propylene process has 99.9% selectivity while the ethylene process starts with 80% - 90% selectivity and decreases over time. Since there are less side products produced, a fuel rich feed can be used without as much worry about losing the propylene supply to side products, which would reduce the yield of the process.

The ethylene process recycles both the oxygen and unreacted ethylene. Since the propylene process is run as a fuel-rich process, there is only a minimal amount of unreacted oxygen in the effluent stream. As a result, the oxygen is discarded rather than recycled. However, the unreacted propylene is recycled and sent back to the reactor.

Pure oxygen was used rather than air in both processes to reduce the volume of inerts in the reactor that would complicate the separation after the reactor to purify the final product.

A contact time of one second was assumed for the propylene process based off the contact time in the ethylene reaction.

The patent describes 100% selectivity of the catalyst in converting propylene to propylene oxide at the operating conditions used in this process. However, no process is 100% selective, so a selectivity of 99.9% was assumed. Because the patent describes 100% selectivity, it does not indicate the side products that can be produced. The side products found in the ethylene to ethylene oxide process were used as a basis for the side products of this process. The combustion reaction forming carbon dioxide and water is the most common side reaction with other reactions producing acetaldehyde, acrolein, and acrylic acid in much smaller quantities. Additionally, there is a further oxidation reaction of propylene oxide that also produces carbon dioxide and water that was also accounted for as in the ethylene process.

The reactor design is similar to that of the ethylene process. A shell and tube reactor is used to double as a heat exchange to capture the energy released from this highly exothermic process. The catalyst is arranged in a packed bed formation with stainless steel tubes in the reactor filled with catalyst supported on a carrier.
6.4 CATALYST REGENERATION

Catalyst supply and detailed background is covered in section 3.3 – *Patent Details and Technology Implementation*. A unique consideration for the oxidation reaction in the process is the relatively quick deactivation time of the catalyst. The catalyst deactivates in around 30 hours, thus making the catalyst regeneration process a priority. The catalyst deactivates because the catalyst reaction process produces carbon, or coke that remains on the catalyst particle and reduces the effectiveness of the catalyst. Regeneration of the catalyst by burning off the coke and the catalyst is prepared for reaction again.\(^1\)

Parallel reactor configuration with regeneration is discussed in section 6.7 – *Reactors in Parallel Configuration*. Both reactors will never be running at the same time, one reactor will be regenerating while one reactor is running. Reactors will switch functions between regeneration and reacting every 24 hours.

The catalyst regeneration process for our design project was based on the fluidized catalytic cracking units (FCCU) that are used in the petroleum industry.\(^2\) These FCCU’s have been used in industry to regenerate catalyst used in the catalytic cracking process. The catalytic cracking process is used to extract additional gasoline from heavier components. Our catalyst regeneration process was based off of theses FCCU’s because of the similar degeneration and coking problems of both processes. The fluidized catalytic cracking unit will continuously route coked catalyst from the inactive reactor during the regeneration cycle of the reactor. While one reactor is regenerating, the other reactor is reacting to produce product. The FCCU routes catalyst into the regenerator unit where oil on the surface of the catalyst is stripped off with either steam or a solvent. The catalyst is sent to the regenerator where the coke is burned off the surface of the catalyst. The continuous catalyst regenerator (CCR) in Figure 3 is a common regenerator, and is the one used in our design process. The optimization of the catalyst regeneration process is necessary to save fuel and to optimize the time of the process. The integral combustor section of the CCR is shown in more detail in Figure 2. The circulation of catalyst in the combustor improves the process of burning coke off the surface of the catalyst. The fractionation step is used to remove the catalyst that has broken into smaller catalyst, so small amounts of catalyst will need to be replaced throughout the regeneration process.\(^2\)
Continuous catalytic regenerator (CRR) utilizes a moving bed process which routes coked and regenerated catalyst. The CRR also controls temperature and oxygen levels in the combustion chamber. The flue gas loop flow rate, temperature, and pressure is regulated by the CRR and the regulation should result in an optimum oxygen concentration and an optimal rate of regeneration.

The complete burn regeneration process in the integral combustor should burn all of the coke off of the catalyst. As shown in Figure 6.2 the flue gasses from this combustion are routed through cleaning equipment then to a flare. The oxygen is measured in this flue gas in order to optimize the combustion process. Oxygen measurements in this step ensure energy is not wasted, and all the coke is being burned.
off of the catalyst. Emerson uses in-situ zirconium-oxide oxygen analyzers in probes similar to ones shown in Figure 6.4. The oxygen probe can gather information on the composition of the flue gas, which should give further information about the real-time efficiency of the regeneration coke burning process. Zirconium oxide oxygen analyzers are the most common in industry today and the main drawback is that they are sensitive to pressure changes. These sensitive oxygen analyzers require special pressure balancing equipment. This equipment is shown in Figure 6.4 and includes a sealed pressure balancing probe which can duplicate process pressure for the probe to regulate readings.21

![Figure 6.4. Pressure Balanced in Situ Oxygen Probe with Isolation Valve](image)

Oxygen probes in for the flue gas in the regenerator can get incorrect readings based on different pressure changes, so a pressure regulator is required for the oxygen probe. These oxygen probes are also placed in the air inlet for the combustion chamber. Oxygen enrichment can increase the efficiency of the entire regeneration process, so pure oxygen is mixed with regeneration air. Oxygen enrichment in a traditional regenerator is shown in Figure 6.5 where an oxygen probe regulates the incoming air. The resulting mixture is slightly higher percent oxygen than ambient air at around 25% oxygen. Oxygen enrichment is shown in Figure 6.2. The oxygen probe is used to monitor and control the oxygen enrichment. The rate of oxygen injection can be monitored and controlled by the oxygen probe.21
Figure 6.5. Traditional Regenerator with Oxygen Enrichment\textsuperscript{21}
6.5 MATERIAL OF CONSTRUCTION

According to the United States Department of Transportation Hazardous Materials Table, propylene oxide is classified as a flammable liquid and hazardous substance. The design of the reactor must take into account the material for the tubes and the material for the shell side. The hazardous materials: propylene oxide, propylene, acrylic acid, acetaldehyde, and acrolein, will only be in contact with the tubes of the reactor. Therefore, the outer shell only has to be designed to accommodate boiler feedwater at the high pressure of 12 bar. To keep the cost down, the outer shell of the heat exchanger will be produced with carbon steel. Water will not have any reactivity with carbon steel so this cheaper metal can be used on the shell side.

For the tube side, stainless steel was chosen for the tubes. Propylene oxide has a high tendency to polymerize when it is in constant contact with steel at high temperatures. Rust buildup on steel tube surfaces could accelerate polymerization of propylene oxide leading to propylene glycols. Carbon steel is susceptible to rust but stainless steel is much more resistant to rusting and corrosion. While stainless steel tubing will increase the cost of the two reactors, the corrosion due to continuous operation will give the reactors a longer lifetime while producing a high quality product.
6.6 REACTORS IN PARALLEL CONFIGURATION

Since the catalyst needs to be regenerated so often, two identical reactors will be used in parallel with only one running at a time. Every twenty-four hours, the valve will be flipped so that the gases all flow into the alternate reactor. During this time, the catalyst will be regenerated in the reactor that had been running for the past day. In a paper titled *Regeneration Kinetics*, R. Hughes and M. Parvinain found that the combustion step in catalyst regeneration was completed in 180-220 minutes. As combustion is the most time consuming step in the regeneration process, the regeneration can easily be completed within the twenty-four hour time frame.

Rather than shut the plant down every day to regenerate the catalyst, this process can run continuously, producing a constant output of propylene oxide every day with the catalyst running at its maximum selectivity and conversion. From an economics standpoint, the additional reactor requires an additional capital investment of only $41,700.
7.0 ENERGY BALANCES AND UTILITIES

7.1 REACTOR ENERGY BALANCE

Heat integration may be considered one of the most important keys to the implementation of this direct oxidation catalyst technology. The direct oxidation is a highly exothermic reaction releasing 114.41 kJ/mol of heat so theoretically speaking, if the reaction was able to achieve 100% conversion, the reaction would yield over 20,000,000 watts of heat. Since the reaction only converts 36.3% of the propylene to propylene oxide, the reaction should theoretically release approximately 7,425,000 watts of heat. There are side products that are produced including water, carbon dioxide, acetaldehyde, acrolein, and acrylic acid but the 99.9% selectivity shows that the majority of the heat is released due to the conversion of propylene to propylene oxide. Therefore, the theoretical heat release would be approximately 7,425,000 watts.

\[
C_3H_6 + \frac{1}{2}O_2 \rightarrow C_3H_6O
\]

\[
H_{\text{formation}}^{C_3H_6} = 20.4 \text{ kJ/mol}
\]

\[
H_{\text{formation}}^{C_3H_6O} = -94.0 \text{ kJ/mol}
\]

\[
\Delta H_{\text{rxn}} = (-94) - (20.4) = -114.4 \text{ kJ/mol}
\]

Equation 7.1. Heat of reaction of the direct oxidation of propylene to propylene oxide

Despite yielding the desired mass flow rates of every component into and out of the reactor, the Aspen simulation resulted in a heat release of only 4,678,700 watts of heat. This is a 37% deviation from the theoretical calculation. A possible reason for the deviation in the calculated heat duty for the reactor is unknown. In terms of the overall process, the lower heat output of the reactor is a safe estimate. The catalyst most likely will not give 36.3% conversion for the total 24 hours of continuous operation. Therefore, the reactor will not be able to release the full theoretical 7,425,000 watts. In addition to the decrease in conversion efficiency as the reactor operates, the reactor will most likely lose some heat to the atmosphere during operation. The 37% decrease in heat released from the theoretical calculation is assumed to be a rough and safe estimate of the heat loss from the reactor. The amount of cooling media pumped in the shell side of the reactor could be manipulated if the reactor heat duty was found to release more than 4,678,700 watts of energy.
7.2 HEAT EXCHANGER ENERGY BALANCES

The two reactors operate at 350°C and 30 bar so the feed material needs to be preheated before it enters the reactors. The E-100 and E-200 heat exchangers are responsible for heating the feeds. Due to the highly exothermic reaction, the reactor needs to be cooled continuously. One way, other than cooling media, to cool the reactor is introduce the feed material colder than the 350°C operating condition. According to industry consultant recommendation, the feed could be introduced to the reactor at 250°C without the risk for huge conversion and selectivity loss.

<table>
<thead>
<tr>
<th>Exchanger</th>
<th>Cold Stream</th>
<th>Inlet T (K)</th>
<th>Outlet T (K)</th>
<th>Mass Flow (mol/s)</th>
<th>( C_p \Delta T (J/mol) )</th>
<th>Theoretical Q (W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-200</td>
<td>OxyFeed</td>
<td>298</td>
<td>523</td>
<td>27.72</td>
<td>7595</td>
<td>210,000</td>
</tr>
<tr>
<td></td>
<td>Pumped P</td>
<td>310</td>
<td>523</td>
<td>151.14</td>
<td>17576</td>
<td>2,656,000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Exchanger</th>
<th>Hot Streams</th>
<th>Inlet T (K)</th>
<th>Outlet T (K)</th>
<th>Mass Flow (mol/s)</th>
<th>Simulated Q (W)</th>
<th>Deviation from Theoretical</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-200</td>
<td>RxnOut</td>
<td>623</td>
<td>612</td>
<td>178.8</td>
<td>193,400</td>
<td>8%</td>
</tr>
<tr>
<td></td>
<td>MidHeat</td>
<td>612</td>
<td>383</td>
<td>178.8</td>
<td>4,717,000</td>
<td>78%</td>
</tr>
</tbody>
</table>

Both the oxygen and propylene feed streams are introduced to the E-200 and E-100 respectively as the cold streams. The reactor effluent has almost 57,500 lb/hr of mostly propylene and propylene oxide at 350°C and is the hot stream in both exchangers. The oxygen and propylene feeds have temperature changes of 225°C and 213°C respectively. Meanwhile, the reactor effluent only drops 11°C through E-200 and 229°C through E-100. The temperature of the reactor effluent proceeding to the initial separation stage is not as important as heating the feed materials so the reactor effluent is able to heat the feed materials without the need to purchase heating utilities.
7.3 UTILITIES

Heat integration throughout the process allows the plant to run very efficiently and allows for every heating utility to be generated by the reactor. Both exchangers and the distillation tower reboilers can be heated using products from the reactor. The reactor needs to be cooled down in order to maintain a constant temperature of 350°C. Based on the calculations in Appendix B, the adiabatic temperature rise in the reactor is 3,510 degrees and somehow the heat produced in the reaction must be captured by a cooling media, in our case boiler feedwater.

<table>
<thead>
<tr>
<th>Table 7.2. Heating and cooling utility usage for process equipment</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Equipment</strong></td>
</tr>
<tr>
<td>R-100/200</td>
</tr>
<tr>
<td>CD-1</td>
</tr>
<tr>
<td>CD-2</td>
</tr>
<tr>
<td>RB-1</td>
</tr>
<tr>
<td>RB-2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Heating Utility Generated</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Equipment</strong></td>
</tr>
<tr>
<td>R-100/200</td>
</tr>
</tbody>
</table>

Overall, the most energy intensive pieces of equipment are CD-1, CD-2 and the reactors, R-100/200. The total amount of cooling utility needed for the condensers and the reactors is 12,576,200 watts. In terms of heating duty for the reboiler, 150lb steam and 50lb steam is needed for RB-1 and RB-2 respectively in order to satisfy a 10°C driving force. Keeping the reactor design in mind, the plant chose to flow the boiler feedwater at a pressure and flow rate that would maintain the water in the liquid state at a very high temperature. The effluent boiler feedwater stream would be at high pressure, 12 bar, and high temperature, 186°C. In order to create 150lb steam, the hot liquid feedwater would enter a flash drum where the pressure would be dropped to 150 psig (10.34 bar) and the temperature kept constant. As a result, the boiler feedwater would be responsible for all of the 150lb steam needed for RB-1 and RB-2.
In order to satisfy a temperature driving force of at least 10° for the 145°C DST-100 bottoms, the steam temperature for RB-1 needs to be above 155°C. Steam is usually sold as either 50lb, 150lb, or 450lb steam with corresponding temperatures of 138°C, 181°C, and 236°C respectively. 50lb steam does not satisfy the desired temperature driving force so 150lb steam is necessary for RB-1. RB-2 only needs 50lb steam because the bottoms temperature of DST-200 is 46°C. However, the reactor is generating 150lb steam for the first reboiler so the 150lb steam can be used for RB-2 as well, generation depicted in Figure 7.1. Based on Table 7.2 above, the reactor can generate 110,361 lb/hr of 150lb steam with the heat released from the reactor and the two distillation reboilers need a total of 22,068 lb/hr of 150lb steam. The reboilers can utilize 22,068 lb/hr giving the process an excess of 88,293 lb/hr of 150lb steam available for the plant to provide as an additional product. Selling the 150lb steam at a rate of $7/1000 lbs would yield almost $4,900,000 per year in strictly steam sales.

In terms of cooling utilities, both the distillation towers, DST-100 and DST-200, have overhead distillates of 41°C and 35°C respectively. Cooling water generally needs at least 5-10 degree driving force so both column condensers can use cooling water assuming a cooling water temperature of 30°C in the gulf coast. Using cooling water is an economically desirable choice and the condensers require almost 25,000 and 33,000 gal/hr of cooling water totaling $5.92/hr or $46,886/year.
Table 7.3. Plant-wide electricity usage for process equipment

<table>
<thead>
<tr>
<th>Equipment</th>
<th>kW</th>
<th>$/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-1</td>
<td>31.27</td>
<td>1.64</td>
</tr>
<tr>
<td>P-2</td>
<td>1.48</td>
<td>0.08</td>
</tr>
<tr>
<td>P-3</td>
<td>28.44</td>
<td>1.49</td>
</tr>
<tr>
<td>RP-1 &amp; RP-2</td>
<td>84.45</td>
<td>4.42</td>
</tr>
<tr>
<td>F-100</td>
<td>61.18</td>
<td>3.20</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>206.82</strong></td>
<td><strong>10.82</strong></td>
</tr>
</tbody>
</table>

Table 7.3 above shows the electricity usage in the entire plant. The flash drum that is responsible for generating the steam at high pressure is the single largest electricity consumer. The flash drum must operate at a high pressure (10.34 bar) and temperature of 181°C to generate the steam. The flash drum in itself costs $25,341 per year in electricity but the steam is sold for almost $4,900,000 per year. The overall cost of the steam generation cycle needs to factor in the 13,248 gal/hr of boiler feedwater at $2/1000 gallons. As a result of the electricity and the boiler feedwater costs, steam generation will result in a profit of $4,664,810 per year.
## 8.0 EQUIPMENT

### 8.1 EQUIPMENT LIST

<table>
<thead>
<tr>
<th>Equipment Number</th>
<th>Name</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pumps</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-1</td>
<td>Centrifugal Pump 1 (propylene)</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>P-2</td>
<td>Centrifugal Pump 2 (recycle)</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>P-3</td>
<td>Centrifugal Pump 3 (BF water)</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Heat Exchanges</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E-100</td>
<td>Heat Exchanger (propylene)</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>E-200</td>
<td>Heat Exchanger (oxygen)</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Reactors</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R-100</td>
<td>Reactor</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>R-200</td>
<td>Reactor</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Adsorber</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A-100</td>
<td>CO$_2$ Adsorber</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Distillation Column Components</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DST-100</td>
<td>Distillation Column 1</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RB-1</td>
<td>DST-100 Reboiler</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RP-1</td>
<td>DST-100 Reflux Pump</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>CD-1</td>
<td>DST-100 Condenser</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RA-1</td>
<td>DST-100 Reflux Accumulator</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>DST-200</td>
<td>Distillation Column 2</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RB-2</td>
<td>DST-100 Reboiler</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RP-2</td>
<td>DST-100 Reflux Pump</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>CD-2</td>
<td>DST-100 Condenser</td>
<td>Process Machinery</td>
</tr>
<tr>
<td>RA-2</td>
<td>DST-100 Reflux Accumulator</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Flash</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F-100</td>
<td>Flash</td>
<td>Process Machinery</td>
</tr>
<tr>
<td><strong>Storage Tank</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T-100</td>
<td>PO Storage Tank</td>
<td>Storage</td>
</tr>
</tbody>
</table>
8.2 UNIT DESCRIPTIONS

8.1.1 PUMPS

**Centrifugal Pump (P-1)**
This pump is installed in the feed pretreatment section of the plant. The pump inlet includes the chemical grade propylene feed and the recycle material stream. The pump is used to get the feed to a high enough pressure to overcome pressure drop until the reactor and to feed the reactor inlets at proper pressure. The discharge pressure of the pump is 32 bar with a volumetric flow rate of 779.2 L/min. The net work required for the pump is 31.27 kW. This pump is process machinery with a purchase cost of $53,100 and a bare module cost of $175,230 calculated from a bare module factor of 3.30.

**Centrifugal Pump (P-2)**
This pump is installed in the initial distillation section of the plant. The pump inlet is the liquid distillate off of distillation tower DST-100. This recycle stream pump is used to pump the recycle to high pressure to be mixed with the propylene inlet feed. This pump is process machinery with a purchase cost of $40,500 and a bare module cost of $133,650 calculated from a bare module factor of 3.30.

**Centrifugal Pump (P-3)**
This pump is installed in the catalytic direct oxidation reaction section of the plant. The pump is used to raise the pressure of the boiler feed water to be fed into the shell side of the reactor. The pressure of the feed water needs to be the same as the reactor tube side pressure. The discharge pressure of the pump is 12 bar with a pressure change of 11 bar and volumetric flow rate of 1010.09 L/min. The net work required is 28.44 kW. This pump is process machinery with a purchase cost of $23,600 and a bare module cost of $77,880 calculated from a bare module factor of 3.30.

8.1.2 HEAT EXCHANGERS

**Heat Exchanger (E-100)**
This heat exchanger is installed in the feed pretreatment section of the plant. It is used to exchange heat between the reactor effluent and the propylene feed. The propylene feed is heated while the reactor effluent is cooled. The reactor effluent goes from 339.22 °C to 109.54 °C and the propylene feed goes from 37.21 °C to 250 °C which is the reactor inlet temperature. The reactor effluent and propylene feed have outlet pressures of 29.70 bar and 31.56 bar, respectively. The heat exchanger has 2 shells in series and 1 shell in parallel with a heat duty of 1,126,849.96 cal/sec and an exchanger area of 106.93 m². Exchanger calculations yielded a UA value of 14,103.30 cal/sec-K and a log mean temperature difference...
of 79.90 °C. This heat exchanger is process machinery with a purchase cost of $57,200 and a bare module cost of $181,324 calculated from a bare module factor of 3.17.

**Heat Exchanger (E-200)**

This heat exchanger is installed in the feed pretreatment section of the plant. It is used to exchange heat between the reactor effluent and the oxygen feed. The oxygen feed is heated while the reactor effluent is cooled. The reactor effluent goes from 350 °C to 339.21 °C and the oxygen feed goes from 37.21 °C to 250 °C which is the reactor inlet temperature. The reactor effluent and oxygen feed have outlet pressures of 29.76 bar and 31.78 bar, respectively. The heat exchanger has 1 shell in series and 1 shell in parallel with a heat duty of 46,257.77 cal/sec and an exchanger area of 2.53 m². Exchanger calculations yielded a UA value of 247.87 cal/sec-K and a log mean temperature difference of 186.62 °C. This heat exchanger is process machinery with a purchase cost of $12,700 and a bare module cost of $40,259 calculated from a bare module factor of 3.17.

8.1.3 REACTORS

**Reactor (R-100)**

This reactor is installed in the catalytic direct oxidation reaction section of the plant. Reactor R-100 and reactor R-200 are in parallel. One reactor is reacting in the process while the other reactor is regenerating. The reactor is a packed bed shell and tube with Ag-W catalyst packed in the tube section. The reactor converts propylene to propylene oxide though direct oxidation and is cooled through suppressed vaporization of boiler feed water in the shell section. This reactor is process machinery with a purchase cost of $13,000 and a bare module cost of $41,730 calculated from a bare module factor of 3.21.

**Reactor (R-200)**

This reactor is installed in the catalytic direct oxidation reaction section of the plant. Reactor R-100 and reactor R-200 are in parallel. One reactor is reacting in the process while the other reactor is regenerating. The reactor is a packed bed shell and tube with Ag-W catalyst packed in the tube section. The reactor converts propylene to propylene oxide though direct oxidation and is cooled through suppressed vaporization of boiler feed water in the shell section. This reactor is process machinery with a purchase cost of $13,000 and a bare module cost of $41,730 calculated from a bare module factor of 3.21.
8.1.4 ADSORBER

**CO₂ Adsorber (A-100)**

The CO₂ adsorber is installed in the initial distillation section of the plant. It is used to remove carbon dioxide from the reactor effluent before distillation. The detailed design of the adsorber is out of this project scope. The adsorber process includes the following equipment: cooler (x3), blower, adsorber, pump (x2), heat exchanger, reboiler, regenerator, compressor and flash drum. This adsorber is responsible for an 80% removal rate of the carbon dioxide in the CO₂Feed stream along with 100% oxygen, 5% water, and 0.00001% propylene removal. The resulting CO₂Out stream will be discharged to the atmosphere. This CO₂ adsorber is process machinery with a purchase cost of $9,806,000 and a bare module cost of $31,477,260 calculated from a bare module factor of 3.21.

8.1.5 DISTILLATION COLUMN COMPONENTS

**Distillation Column (DST-100)**

This distillation column is installed in the initial distillation section of the plant after the CO₂ remover. This column is used to separate out the propylene from the reactor effluent product mixture. The tower manages to achieve a split of 99.975% of propylene into the distillate and 99.923% of propylene oxide into the bottoms. The column is 2-phase with 23 stages, a reflux ratio of 3.563, and a calculated molar reflux ratio of 1.778. The condenser top stage temperature is 40.98 °C with a pressure of 17 bar. The distillation column has a bottoms rate of 197.97 kmol/hr and a distillate rate of 346.49 kmol/hr. This distillation column is process machinery with a purchase cost of $180,200 and a bare module cost of $578,422 calculated from a bare module factor of 3.21.

**DST-100 Reboiler (RB-1)**

This reboiler is part of DST-100 and is installed in the initial distillation section of the plant. The reboiler uses steam utility from the steam created from the reactor cooling section. The reboiler takes liquid from bottoms product and returns it to the distillation column as vapor. The reboiler is a kettle type reboiler with a boilup rate of 361.19 kmol/hr. The reboiler pressure is 17 bar and temperature is 145.09 °C. The heat duty of the reboiler is 468,135.90 cal/sec which uses 3467.73 kg/hr of steam at a rate of 15.52$/hr. This reboiler is process machinery with a purchase cost of $38,300 and a bare module cost of $122,943 calculated from a bare module factor of 3.21.

**DST-100 Reflux Pump (RP-1)**

This reflux pump is part of DST-100 and is installed in the initial distillation section of the plant. The pump helps control the flow of reflux from the distillate back into the column. The reflux pump maintains
the reflux ratio of 3.5628, and calculated molar reflux ratio of 1.77. This reflux pump is process machinery with a purchase cost of $8,400 and a bare module cost of $27,720 calculated from a bare module factor of 3.30.

**DST-100 Condenser (CD-1)**
This condenser is part of DST-100 and is installed in the initial distillation section of the plant. The condenser, CD-1, was chosen to operate at a pressure of 17 bar in order for the condenser to utilize cooling water as the cooling media instead of an expensive refrigerant. Condenser duty is negative 815,874.66 cal/sec and has reflux rate of 615.67 kmol/hr. It uses 589,068.56 kg/hr of cooling water at a rate of 2.61 $/hr. This condenser is process machinery with a purchase cost of $65,900 and a bare module cost of $211,539 calculated from a bare module factor of 3.21.

**DST-100 Reflux Accumulator (RA-1)**
This reflux accumulator is part of DST-100 and is installed in the initial distillation section of the plant. This accumulator helps control the flow of reflux and product. The reflux accumulator maintains the reflux ratio of 3.5628, and calculated molar reflux ratio of 1.77. This reflux accumulator is process machinery with a purchase cost of $29,300 and a bare module cost of $94,053 calculated from a bare module factor of 3.21.

**Distillation Column (DST-200)**
This distillation column is installed in the final distillation section of the plant. The tower separates the process stream into a liquid product stream and a waste stream. The feed from the initial distillation into DST-200 contains water, acrylic acid, acetaldehyde, propylene, and mostly propylene oxide. DST-200 separates out impurities from the propylene oxide to meet product specifications. The column is 2-phase with 14 stages, a reflux ratio of 2, and a calculated molar reflux ratio of 2. The condenser top stage temperature is 34.06 °C with a pressure of 1 bar. The distillation column has a bottoms rate of 0.534 kmol/hr and a distillate rate of 197.43 kmol/hr. This distillation column is process machinery with a purchase cost of $139,100 and a bare module cost of $446,511 calculated from a bare module factor of 3.21.

**DST-200 Reboiler (RB-2)**
This reboiler is part of DST-200 and is installed in the initial distillation section of the plant. The reboiler uses steam utility from the steam created from the reactor cooling section. The reboiler takes liquid from bottoms product and returns it to the distillation column as vapor. The reboiler is a kettle type reboiler.
with a boilup rate of 447.95 kmol/hr. The reboiler pressure is 1 bar and temperature is 46.30 °C. The heat
duty of the reboiler is 868,528.958 cal/sec which uses 5972.45 kg/hr of steam at a rate of 24.87$/hr. This
reboiler is process machinery with a purchase cost of $21,500 and a bare module cost of $69,015
calculated from a bare module factor of 3.21.

**DST-200 Reflux Pump (RP-2)**
This reflux pump is part of DST-100 and is installed in the initial distillation section of the plant. The pump helps control the flow of reflux from the distillate back into the column. The reflux pump maintains the reflux ratio of 2, and calculated molar reflux ratio of 2. This reflux pump is process machinery with a purchase cost of $6,800 and a bare module cost of $22,440 calculated from a bare module factor of 3.30.

**DST-200 Condenser (CD-2)**
This condenser is part of DST-100 and is installed in the initial distillation section of the plant. The condenser, at atmospheric temperature, can utilize cooling water as the cooling media instead of an expensive refrigerant. Condenser duty is negative -1,070,418.02 cal/sec and has reflux rate of 394.86 kmol/hr. It uses 772,851.066 kg/hr of cooling water at a rate of 3.42 $/hr. This condenser is process machinery with a purchase cost of $98,800 and a bare module cost of $317,148 calculated from a bare module factor of 3.21.

**DST-200 Reflux Accumulator (RA-2)**
This reflux accumulator is part of DST-100 and is installed in the initial distillation section of the plant. This accumulator helps control the flow of reflux and product. The reflux accumulator maintains the reflux ratio of 2, and calculated molar reflux ratio of 2. This reflux accumulator is process machinery with a purchase cost of $20,600 and a bare module cost of $66,126 calculated from a bare module factor of 3.21.

8.1.6 FLASH

**Flash (F-100)**
The flash drum is installed in the reactor cycle section of the plant. The drum is used to lower the pressure of the hot water outlet from the shell side of the reactor in order to vaporize the water and make steam. The drum is part of the suppressed vaporization process used to cool the reactor and make steam. The outlet temperature of the drum is 181.35 °C and the outlet pressure is 10.32 bar. The heat duty of the drum is 6,664,356.08 cal/sec. This flash drum is process machinery with a purchase cost of $31,500 and a bare module cost of $101,115 calculated from a bare module factor of 3.21.
8.1.7 STORAGE TANK

*PO Storage Tank (T-100)*

The storage tank for propylene oxide product is installed in the final distillation section of the plant. The tank is used to store propylene oxide product for testing and distribution. This storage tank is storage type with a purchase cost of $430,900 and a bare module cost of $1,383,189 calculated from a bare module factor of 3.21.
## 8.3 UNIT SPECIFICATIONS

### 8.3.1 PUMPS

<table>
<thead>
<tr>
<th>P-1</th>
<th>Equipment</th>
<th>Pump</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Stream</td>
<td>Mixed</td>
<td></td>
</tr>
<tr>
<td>Outlet Stream</td>
<td>Pump</td>
<td></td>
</tr>
<tr>
<td><strong>Function</strong></td>
<td>Pump mix of feed and recycled propylene from M-1</td>
<td></td>
</tr>
<tr>
<td><strong>Type</strong></td>
<td>Centrifugal Pump</td>
<td></td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Efficiency (%)</td>
<td>0.623</td>
<td>Inlet Pressure (bar)</td>
</tr>
<tr>
<td>Casting Material</td>
<td>Carbon Steel</td>
<td>Outlet Pressure (bar)</td>
</tr>
<tr>
<td>Fluid Head (M-kgf/kg)</td>
<td>312</td>
<td>Net Work (kW)</td>
</tr>
<tr>
<td>Liquid Flow Rate (L/min)</td>
<td>779.2</td>
<td>Electricity (kW)</td>
</tr>
<tr>
<td>Installed Weight (lbs)</td>
<td>8437</td>
<td></td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>Purchase (USD)</td>
<td>$53,100</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>P-2</th>
<th>Equipment</th>
<th>Pump</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Stream</td>
<td>DistLiq1</td>
<td></td>
</tr>
<tr>
<td>Outlet Stream</td>
<td>Recycle</td>
<td></td>
</tr>
<tr>
<td><strong>Function</strong></td>
<td>Pump the recycle stream to a higher pressure to be mixed with propylene feed</td>
<td></td>
</tr>
<tr>
<td><strong>Type</strong></td>
<td>Centrifugal</td>
<td></td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Efficiency (%)</td>
<td>0.572</td>
<td>Inlet Pressure (bar)</td>
</tr>
<tr>
<td>Casting Material</td>
<td>Carbon Steel</td>
<td>Outlet Pressure (bar)</td>
</tr>
<tr>
<td>Fluid Head (M-kgf/kg)</td>
<td>21.3</td>
<td>Net Work (kW)</td>
</tr>
<tr>
<td>Liquid Flow Rate (L/min)</td>
<td>507</td>
<td>Electricity (kW)</td>
</tr>
<tr>
<td>Installed Weight (lbs)</td>
<td>4836</td>
<td></td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>Purchase (USD)</td>
<td>$40,500</td>
</tr>
</tbody>
</table>
### Identification

**Equipment**: Pump  
**Inlet Stream**: BFWaterIn  
**Outlet Stream**: HotWater

**Function**: Pumps the boiler feed water through the system  
**Type**: Centrifugal Pump

<table>
<thead>
<tr>
<th>Design</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Efficiency (%)</td>
<td>0.651</td>
</tr>
<tr>
<td>Casting Material</td>
<td>Carbon Steel</td>
</tr>
<tr>
<td>Fluid Head (M-kGF/kg)</td>
<td>136</td>
</tr>
<tr>
<td>Liquid Flow Rate (L/min)</td>
<td>1010</td>
</tr>
<tr>
<td>Installed Weight (lbs)</td>
<td>8650</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchase (USD)</td>
<td>$23,600</td>
</tr>
<tr>
<td>Bare Module (USD)</td>
<td>$77,880</td>
</tr>
</tbody>
</table>

### 8.3.2 HEAT EXCHANGERS

#### E-100

**Identification**  
**Equipment**: Heat Exchanger  
**Inlet Stream**: PumpedP  
**Outlet Stream**: PropIn

**Function**: Heat up propylene feed while cooling reactor effluent  
**Type**: Shell and Tube Heat Exchanger

<table>
<thead>
<tr>
<th>Design</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exchange Area (ft²)</td>
<td>586</td>
</tr>
<tr>
<td>Tube Temperature (deg C)</td>
<td>155</td>
</tr>
<tr>
<td>Shell Temperature (deg C)</td>
<td>127</td>
</tr>
<tr>
<td>Tube Pitch (in)</td>
<td>1.41</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchase (USD)</td>
<td>$57,200</td>
</tr>
<tr>
<td>Bare Module (USD)</td>
<td>$181,324</td>
</tr>
</tbody>
</table>

#### E-200

**Identification**  
**Equipment**: Heat Exchanger  
**Inlet Stream**: OxyFeed  
**Outlet Stream**: OxIn

**Function**: Heat up oxygen feed while cooling reactor effluent  
**Type**: Shell and Tube Heat Exchanger

<table>
<thead>
<tr>
<th>Design</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exchange Area (ft²)</td>
<td>29.0</td>
</tr>
<tr>
<td>Tube Temperature (deg C)</td>
<td>311</td>
</tr>
<tr>
<td>Shell Temperature (deg C)</td>
<td>155</td>
</tr>
<tr>
<td>Tube Pitch (in)</td>
<td>1.875</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchase (USD)</td>
<td>$12,700</td>
</tr>
<tr>
<td>Bare Module (USD)</td>
<td>$40,259</td>
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### 8.3.3 REACTORS

<table>
<thead>
<tr>
<th>Identification</th>
<th>Reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Stream</td>
<td>PropIn, OxIn</td>
</tr>
<tr>
<td>Outlet Stream</td>
<td>RxnOut</td>
</tr>
</tbody>
</table>

**Main Reactions**
- Propylene + 0.5 Oxygen $\rightarrow$ Propylene Oxide

**Side Reactions**
- $2 \text{ Propylene} + 9 \text{ Oxygen} \rightarrow 6 \text{ Carbon Dioxide} + 6 \text{ Water}$
- $2 \text{ Propylene} + 1.5 \text{ Oxygen} \rightarrow 3 \text{ Acetaldehyde}$
- Propylene + Oxygen $\rightarrow$ Acrolein + Water
- Propylene + 1.5 Oxygen $\rightarrow$ Acrylic Acid + Water
- Propylene Oxide + 4 Oxygen $\rightarrow$ 3 Carbon Dioxide + 3 Water

**Classification**
- Shell and tube

**Design**
- Temperature (deg C): 350
- Pressure (bar): 30
- Construction Material: Carbon Steel
- Heat Duty (kcal/s): 1120

**Component Flow Rates (kg/hr)**

<table>
<thead>
<tr>
<th>Component</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propylene</td>
<td>22900</td>
<td>14600</td>
</tr>
<tr>
<td>Acrolein</td>
<td>1.21E-07</td>
<td>0.443</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>8.85</td>
<td>11500</td>
</tr>
<tr>
<td>Oxygen</td>
<td>3190</td>
<td>8.89</td>
</tr>
<tr>
<td>Water</td>
<td>3.73E-12</td>
<td>9.67</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>5.73</td>
<td>28.7</td>
</tr>
<tr>
<td>Acetaldehyde</td>
<td>1.02E-04</td>
<td>0.522</td>
</tr>
<tr>
<td>Acrylic Acid</td>
<td>5.80E-18</td>
<td>0.569</td>
</tr>
</tbody>
</table>

**Cost**
- Purchase (USD): $28,600
- Bare Module (USD): $90,662
- Cost of Catalyst (USD): $4,600
- Total Bare Module (USD): $95,262
<table>
<thead>
<tr>
<th>Identification</th>
<th>Equipment</th>
<th>Reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Stream</td>
<td>PropIn2, OxIn2</td>
<td></td>
</tr>
<tr>
<td>Outlet Stream</td>
<td>RxnOut</td>
<td></td>
</tr>
<tr>
<td><strong>Main Reactions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene + 0.5 Oxygen --&gt; Propylene Oxide</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Side Reactions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 Propylene + 9 Oxygen --&gt; 6 Carbon Dioxide + 6 Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 Propylene + 1.5 Oxygen --&gt; 3 Acetaldehyde</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene + Oxygen --&gt; Acrolein + Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene + 1.5 Oxygen --&gt; Acrylic Acid + Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene Oxide + 4 Oxygen --&gt; 3 Carbon Dioxide + 3 Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Classification</strong></td>
<td>Shell and tube</td>
<td></td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature (deg C)</td>
<td>350</td>
<td>Carbon Steel</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>30</td>
<td>-1120</td>
</tr>
<tr>
<td><strong>Component Flow Rates (kg/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene</td>
<td>22900</td>
<td>14600</td>
</tr>
<tr>
<td>Acrolein</td>
<td>1.21E-07</td>
<td>0.443</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>8.85</td>
<td>11500</td>
</tr>
<tr>
<td>Oxygen</td>
<td>3190</td>
<td>8.89</td>
</tr>
<tr>
<td>Water</td>
<td>3.73E-12</td>
<td>9.67</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>5.73</td>
<td>28.7</td>
</tr>
<tr>
<td>Acetaldehyde</td>
<td>1.02E-04</td>
<td>0.522</td>
</tr>
<tr>
<td>Acrylic Acid</td>
<td>5.80E-18</td>
<td>0.569</td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Purchase (USD)</td>
<td>$28,600</td>
<td>Bare Module (USD)</td>
</tr>
<tr>
<td>Cost of Catalyst (USD)</td>
<td>$4,600</td>
<td>Total Bare Module (USD)</td>
</tr>
</tbody>
</table>
### 8.3.4. ADSORBER

<table>
<thead>
<tr>
<th>Identification</th>
<th>Equipment</th>
<th>Adsorber</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>Remove CO2 and oxygen from the reactor effluent</td>
<td></td>
</tr>
<tr>
<td><strong>Materials</strong></td>
<td>Feed</td>
<td>CO2 Out</td>
</tr>
<tr>
<td>Stream ID</td>
<td>CO2Feed</td>
<td>CO2Out</td>
</tr>
<tr>
<td>Temperature (deg C)</td>
<td>109.5</td>
<td>109.5</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>29.7</td>
<td>29.7</td>
</tr>
<tr>
<td>Total Flow Rate (kg/hr)</td>
<td>26090</td>
<td>32.3</td>
</tr>
<tr>
<td><strong>Component Flow Rates (kg/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene</td>
<td>14600</td>
<td>0.0146</td>
</tr>
<tr>
<td>Acrolein</td>
<td>0.443</td>
<td>0</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>11500</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>8.89</td>
<td>8.89</td>
</tr>
<tr>
<td>Water</td>
<td>9.67</td>
<td>0.484</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>28.7</td>
<td>22.9</td>
</tr>
<tr>
<td>Acetaldehyde</td>
<td>0.522</td>
<td>0</td>
</tr>
<tr>
<td>Acrylic Acid</td>
<td>0.569</td>
<td>0</td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>Purchase (USD)</td>
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### 8.3.5 DISTILLATION COLUMNS

#### DST-100

<table>
<thead>
<tr>
<th>Identification</th>
<th>Equipment</th>
<th>Distillation Column</th>
</tr>
</thead>
<tbody>
<tr>
<td>Function</td>
<td></td>
<td>Remove propylene for recycle</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Design</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Trays</td>
<td>23</td>
<td></td>
</tr>
<tr>
<td>Total Weight (lbs)</td>
<td>172000</td>
<td></td>
</tr>
<tr>
<td>Feed Stage</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>Total Height (m)</td>
<td>22.6</td>
<td></td>
</tr>
<tr>
<td>Construction Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Condenser Pressure (bar)</td>
<td>17</td>
<td></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Materials</th>
<th>Feed</th>
<th>Liquid Distillate</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream ID</td>
<td>Sep Feed</td>
<td>DistLiq1</td>
<td>Bottoms1</td>
</tr>
<tr>
<td>Temperature (deg C)</td>
<td>110</td>
<td>41</td>
<td>145</td>
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<tr>
<td>Pressure (bar)</td>
<td>29.7</td>
<td>17</td>
<td>17</td>
</tr>
<tr>
<td>Total Flow Rate (kg/hr)</td>
<td>26060</td>
<td>14600</td>
<td>11500</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component Flow Rates (kg/hr)</th>
<th>Propylene</th>
<th>Acrolein</th>
<th>Propylene Oxide</th>
<th>Water</th>
<th>Carbon Dioxide</th>
<th>Acetaldehyde</th>
<th>Acrylic Acid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>14600</td>
<td>0.443</td>
<td>11500</td>
<td>9.19</td>
<td>5.73</td>
<td>0.522</td>
<td>0.569</td>
</tr>
<tr>
<td></td>
<td>11500</td>
<td>11500</td>
<td>8.85</td>
<td>3.83E-12</td>
<td>5.73</td>
<td>11500</td>
<td>5.93E-18</td>
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<table>
<thead>
<tr>
<th>Cost</th>
<th>Purchase (USD)</th>
<th>Bare Module (USD)</th>
</tr>
</thead>
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<tr>
<td></td>
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### DST-200

<table>
<thead>
<tr>
<th>Identification</th>
<th>Equipment</th>
<th>Distillation Column</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>Remove impurities to purify propylene oxide product</td>
<td></td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td>Number of Trays</td>
<td>14</td>
</tr>
<tr>
<td></td>
<td>Column Diameter (m)</td>
<td>1.98</td>
</tr>
<tr>
<td></td>
<td>Total Weight (lbs)</td>
<td>158000</td>
</tr>
<tr>
<td></td>
<td>Tray Spacing (m)</td>
<td>0.61</td>
</tr>
<tr>
<td></td>
<td>Feed Stage</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>Tray Type</td>
<td>Sieve</td>
</tr>
<tr>
<td></td>
<td>Total Height (m)</td>
<td>14.6</td>
</tr>
<tr>
<td></td>
<td>Condenser Duty (kcal/s)</td>
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</tr>
<tr>
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<td>Construction Material</td>
<td>Carbon Steel</td>
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<td></td>
<td>Condenser Pressure (bar)</td>
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<tr>
<td></td>
<td>Reflux Ratio</td>
<td>2.00</td>
</tr>
<tr>
<td><strong>Materials</strong></td>
<td>Stream ID</td>
<td>Feed</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Liquid Distillate</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Bottoms</td>
</tr>
<tr>
<td></td>
<td>Temperature (deg C)</td>
<td>SepFeed2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>34.2</td>
</tr>
<tr>
<td></td>
<td>Pressure (bar)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Total Flow Rate (kg/hr)</td>
<td>11480</td>
</tr>
<tr>
<td><strong>Component Flow Rates (kg/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Propylene</td>
<td>0.754</td>
<td>0.754</td>
</tr>
<tr>
<td>Acrolein</td>
<td>0.443</td>
<td>0.380</td>
</tr>
<tr>
<td>Propylene Oxide</td>
<td>11466</td>
<td>11464</td>
</tr>
<tr>
<td>Water</td>
<td>9.19</td>
<td>0.387</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>6.65E-07</td>
<td>6.65E-07</td>
</tr>
<tr>
<td>Acetaldehyde</td>
<td>0.522</td>
<td>0.522</td>
</tr>
<tr>
<td>Acrylic Acid</td>
<td>0.569</td>
<td>4.12E-12</td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>Purchase (USD)</td>
<td>$286,700</td>
</tr>
<tr>
<td></td>
<td>Bare Module (USD)</td>
<td>$920,919</td>
</tr>
</tbody>
</table>

8.3.6 FLASH DRUM

<table>
<thead>
<tr>
<th>F-100</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
<td>Equipment</td>
<td>Flash Vessel</td>
</tr>
<tr>
<td></td>
<td>Inlet Stream</td>
<td>HotWater</td>
</tr>
<tr>
<td></td>
<td>Overhead</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td>Bottoms</td>
<td>SteamOut</td>
</tr>
<tr>
<td><strong>Function</strong></td>
<td>Turn already heated water into steam</td>
<td></td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td>Temperature (deg C)</td>
<td>182</td>
</tr>
<tr>
<td></td>
<td>Pressure (bar)</td>
<td>10.3</td>
</tr>
<tr>
<td></td>
<td>Bottoms Flow Rate (kg/hr)</td>
<td>50060</td>
</tr>
<tr>
<td></td>
<td>Vapor Flow Rate (kg/hr)</td>
<td>50060</td>
</tr>
<tr>
<td></td>
<td>Liquid Volume (L)</td>
<td>12000</td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>Purchase (USD)</td>
<td>$31,500</td>
</tr>
<tr>
<td></td>
<td>Bare Module (USD)</td>
<td>$101,115</td>
</tr>
</tbody>
</table>
### 8.3.7 STORAGE TANK

<table>
<thead>
<tr>
<th><strong>Identification</strong></th>
<th><strong>T-100</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Equipment</td>
<td>Storage Tank</td>
</tr>
<tr>
<td>Inlet Stream</td>
<td>Product</td>
</tr>
<tr>
<td>Outlet Stream</td>
<td>ProductOut</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Function</strong></th>
<th>Store the manufactured propylene oxide</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Classification</strong></td>
<td>Floating roof tank</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Design</strong></th>
<th><strong>Value</strong></th>
<th><strong>Value</strong></th>
<th><strong>Value</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacity (gal)</td>
<td>630000</td>
<td>Residence Time</td>
<td>7 days</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.00</td>
<td>Construction Material</td>
<td>Stainless Steel</td>
</tr>
<tr>
<td>Temperature (deg C)</td>
<td>34.1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Cost</strong></th>
<th><strong>Value</strong></th>
<th><strong>Value</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchase (USD)</td>
<td>$431,000</td>
<td>Bare Module (USD)</td>
</tr>
</tbody>
</table>
9.0 COSTING

9.1 EQUIPMENT COST SUMMARY

Table 9.1 shows the equipment description, type of equipment, purchase cost, and bare module cost for each piece of equipment in the process. The purchase cost for each piece of equipment was found through ASPEN IPE except for the reactors, heat exchangers, catalyst and the CO2 adsorber. The size and cost of the reactors and heat exchangers were found by using the methods in Seider et al. The cost of the catalyst was calculated using a price of $50 per pound. The cost of the CO2 adsorber was found by studying similar systems as the design of the CO2 adsorber is outside the scope of this project.

<table>
<thead>
<tr>
<th>Equipment Description</th>
<th>Type</th>
<th>Purchase Cost</th>
<th>Bare Module Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pump P-1</td>
<td>Process Machinery</td>
<td>$53,100</td>
<td>$175,230</td>
</tr>
<tr>
<td>Recycle Pump P-2</td>
<td>Process Machinery</td>
<td>$40,500</td>
<td>$133,650</td>
</tr>
<tr>
<td>Pump P-3</td>
<td>Process Machinery</td>
<td>$23,600</td>
<td>$77,880</td>
</tr>
<tr>
<td>Heat Exchanger E-100</td>
<td>Fabricated Equipment</td>
<td>$57,200</td>
<td>$181,324</td>
</tr>
<tr>
<td>Heat Exchanger E-200</td>
<td>Fabricated Equipment</td>
<td>$12,700</td>
<td>$40,259</td>
</tr>
<tr>
<td>Reactor R-100</td>
<td>Fabricated Equipment</td>
<td>$28,600</td>
<td>$90,662</td>
</tr>
<tr>
<td>Reactor R-200</td>
<td>Fabricated Equipment</td>
<td>$28,600</td>
<td>$90,662</td>
</tr>
<tr>
<td>CO2 Adsorber A-100</td>
<td>Fabricated Equipment</td>
<td>$9,806,000</td>
<td>$31,477,260</td>
</tr>
<tr>
<td>Distillation Column DST-100</td>
<td>Fabricated Equipment</td>
<td>$180,000</td>
<td>$577,800</td>
</tr>
<tr>
<td>Reboiler RB-1</td>
<td>Fabricated Equipment</td>
<td>$38,300</td>
<td>$122,943</td>
</tr>
<tr>
<td>Reflux Pump RP-1</td>
<td>Fabricated Equipment</td>
<td>$8,400</td>
<td>$27,720</td>
</tr>
<tr>
<td>Condenser CD-1</td>
<td>Fabricated Equipment</td>
<td>$65,900</td>
<td>$211,539</td>
</tr>
<tr>
<td>Reflux Accumulator RA-1</td>
<td>Fabricated Equipment</td>
<td>$29,300</td>
<td>$94,053</td>
</tr>
<tr>
<td>Distillation Column DST-200</td>
<td>Fabricated Equipment</td>
<td>$139,000</td>
<td>$446,190</td>
</tr>
<tr>
<td>Reboiler RB-2</td>
<td>Fabricated Equipment</td>
<td>$21,500</td>
<td>$69,015</td>
</tr>
<tr>
<td>Reflux Pump RP-2</td>
<td>Fabricated Equipment</td>
<td>$6,800</td>
<td>$22,440</td>
</tr>
<tr>
<td>Condenser CD-2</td>
<td>Fabricated Equipment</td>
<td>$98,800</td>
<td>$317,148</td>
</tr>
<tr>
<td>Reflux Accumulator RA-2</td>
<td>Fabricated Equipment</td>
<td>$20,600</td>
<td>$66,126</td>
</tr>
<tr>
<td>------------------------</td>
<td>----------------------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>Flash F-100</td>
<td>Fabricated Equipment</td>
<td>$31,500</td>
<td>$101,115</td>
</tr>
<tr>
<td>Catalyst for R-100</td>
<td>Catalysts</td>
<td>$4,600</td>
<td>$4,600</td>
</tr>
<tr>
<td>Catalyst for R-200</td>
<td>Catalysts</td>
<td>$4,600</td>
<td>$4,600</td>
</tr>
<tr>
<td>PO Storage Tank</td>
<td>Storage</td>
<td>$431,000</td>
<td>$1,383,510</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td></td>
<td><strong>$11,130,600</strong></td>
<td><strong>$35,715,726</strong></td>
</tr>
</tbody>
</table>

### 9.2 OVERALL COST AND INVESTMENT SUMMARY

Table 9.2 shows the cost and investment summary for the process. The current year, 2016, is used for finalizing plans for the project. The permanent investment is all made in 2017, the year of construction. After construction, the plant operates at 45% capacity for its first year, 67.5% capacity for its second year, and finally at 90% capacity for thirteen years after that until the plant is permanently shut down and parts sold.

There is a total capital investment of approximately $63 million, of which approximately $52 million is a permanent investment. The other investment comes from variable costs, mostly the supply of oxygen and propylene needed for the process.

Additional permanent investment costs were calculated as a percentage of total bare module costs and then of the direct permanent investment and total depreciable capital. Fixed costs include total permanent investment along with operations, maintenance, operating overhead, taxes, and depreciation.

Variable costs primarily include the cost of the raw materials, oxygen and propylene. Other variable costs include general expenses, such as sales expenses, research, administrative expenses, and management incentives. These were calculated as a percentage of sales.
### Table 9.2. Cost and Investment Summary

#### Variable Cost Summary

**Variable Costs at 100% Capacity:**

**General Expenses**

<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Selling / Transfer Expenses</td>
<td>$6,809,813</td>
</tr>
<tr>
<td>Direct Research</td>
<td>$10,895,701</td>
</tr>
<tr>
<td>Allocated Research</td>
<td>$1,134,969</td>
</tr>
<tr>
<td>Administrative Expense</td>
<td>$4,539,875</td>
</tr>
<tr>
<td>Management Incentive Compensation</td>
<td>$2,837,422</td>
</tr>
</tbody>
</table>

**Total General Expenses** $26,217,780

<table>
<thead>
<tr>
<th>Raw Materials</th>
<th>$0.381170 per lb of Propylene Oxide</th>
<th>$76,299,063</th>
</tr>
</thead>
<tbody>
<tr>
<td>Byproducts</td>
<td>$0.022937 per lb of Propylene Oxide</td>
<td>($4,591,327)</td>
</tr>
<tr>
<td>Utilities</td>
<td>$0.001506 per lb of Propylene Oxide</td>
<td>$301,506</td>
</tr>
</tbody>
</table>

**Total Variable Costs** $98,227,022

#### Fixed Cost Summary

**Operations**

<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct Wages and Benefits</td>
<td>$416,000</td>
</tr>
<tr>
<td>Direct Salaries and Benefits</td>
<td>$62,400</td>
</tr>
<tr>
<td>Operating Supplies and Services</td>
<td>$24,960</td>
</tr>
<tr>
<td>Technical Assistance to Manufacturing</td>
<td>$300,000</td>
</tr>
<tr>
<td>Control Laboratory</td>
<td>$325,000</td>
</tr>
</tbody>
</table>

**Total Operations** $1,128,360

**Maintenance**
<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wages and Benefits</td>
<td>$2,086,156</td>
</tr>
<tr>
<td>Salaries and Benefits</td>
<td>$521,539</td>
</tr>
<tr>
<td>Materials and Services</td>
<td>$2,086,156</td>
</tr>
<tr>
<td>Maintenance Overhead</td>
<td>$104,308</td>
</tr>
<tr>
<td><strong>Total Maintenance</strong></td>
<td><strong>$4,798,158</strong></td>
</tr>
</tbody>
</table>

**Operating Overhead**

- General Plant Overhead: $219,113
- Mechanical Department Services: $74,066
- Employee Relations Department: $182,080
- Business Services: $228,371

**Total Operating Overhead** $703,630

**Property Taxes and Insurance**

- Property Taxes and Insurance: $927,180

**Other Annual Expenses**

- Rental Fees (Office and Laboratory Space): $
- Licensing Fees: $
- Miscellaneous: $

**Total Other Annual Expenses** $

**Total Fixed Costs** $7,557,328
## Investment Summary

**Total Bare Module Costs:**

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabricated Equipment</td>
<td>$33,936,256</td>
</tr>
<tr>
<td>Process Machinery</td>
<td>$386,760</td>
</tr>
<tr>
<td>Spares</td>
<td>$-</td>
</tr>
<tr>
<td>Storage</td>
<td>$1,383,510</td>
</tr>
<tr>
<td>Other Equipment</td>
<td>$-</td>
</tr>
<tr>
<td>Catalysts</td>
<td>$9,200</td>
</tr>
<tr>
<td>Computers, Software, Etc.</td>
<td>$-</td>
</tr>
</tbody>
</table>

**Total Bare Module Costs:** $35,715,726

**Direct Permanent Investment**

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Site Preparations:</td>
<td>$1,785,786</td>
</tr>
<tr>
<td>Cost of Service Facilities:</td>
<td>$1,785,786</td>
</tr>
<tr>
<td>Allocated Costs for utility plants and related facilities:</td>
<td>$-</td>
</tr>
</tbody>
</table>

**Direct Permanent Investment** $39,287,299

**Total Depreciable Capital**

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Contingencies &amp; Contractor Fees</td>
<td>$7,071,714</td>
</tr>
</tbody>
</table>

**Total Depreciable Capital** $46,359,012

**Total Permanent Investment**

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Land:</td>
<td>$927,180</td>
</tr>
<tr>
<td>Cost of Royalties:</td>
<td>$-</td>
</tr>
<tr>
<td>Cost of Plant Start-Up:</td>
<td>$4,635,901</td>
</tr>
</tbody>
</table>

**Total Permanent Investment - Unadjusted** $51,922,094
### Site Factor
Total Permanent Investment: 1.00 $51,922,094

### Working Capital

<table>
<thead>
<tr>
<th></th>
<th>2017</th>
<th>2018</th>
<th>2019</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accounts Receivable</td>
<td>$8,395,660</td>
<td>$4,197,830</td>
<td>$4,197,830</td>
</tr>
<tr>
<td>Cash Reserves</td>
<td>$290,669</td>
<td>$145,335</td>
<td>$145,335</td>
</tr>
<tr>
<td>Accounts Payable</td>
<td>$(2,833,172)</td>
<td>$(1,416,586)</td>
<td>$(1,416,586)</td>
</tr>
<tr>
<td>Propylene Oxide Inventory</td>
<td>$1,119,421</td>
<td>$559,711</td>
<td>$559,711</td>
</tr>
<tr>
<td>Raw Materials</td>
<td>$188,135</td>
<td>$94,067</td>
<td>$94,067</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$7,160,713</strong></td>
<td><strong>$3,580,357</strong></td>
<td><strong>$3,580,357</strong></td>
</tr>
</tbody>
</table>

*Present Value at 15%*

<table>
<thead>
<tr>
<th></th>
<th>2017</th>
<th>2018</th>
<th>2019</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$6,226,707</td>
<td>$2,707,264</td>
<td>$2,354,143</td>
</tr>
</tbody>
</table>

**Total Capital Investment** $63,210,208
Table 9.3. General Information

<table>
<thead>
<tr>
<th>Process Title:</th>
<th>Propylene to Propylene Oxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product:</td>
<td>Propylene Oxide</td>
</tr>
<tr>
<td>Plant Site Location:</td>
<td>United States Gulf Coast</td>
</tr>
<tr>
<td>Site Factor:</td>
<td>1.00</td>
</tr>
<tr>
<td>Operating Hours per Year:</td>
<td>7919</td>
</tr>
<tr>
<td>Operating Days Per Year:</td>
<td>330</td>
</tr>
<tr>
<td>Operating Factor:</td>
<td>0.9040</td>
</tr>
</tbody>
</table>

**Product Information**

This Process will Yield

- 25,277 lb of Propylene Oxide per hour
- 606,652 lb of Propylene Oxide per day
- 200,170,872 lb of Propylene Oxide per year

**Price**

$1.13 /lb

**Chronology**

<table>
<thead>
<tr>
<th>Year</th>
<th>Action</th>
<th>Distribution of Permanent Investment</th>
<th>Production Capacity</th>
<th>Depreciation 5 year MACRS</th>
<th>Product Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>2016</td>
<td>Design</td>
<td>0.0%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2017</td>
<td>Construction</td>
<td>100%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2018</td>
<td>Production</td>
<td>0%</td>
<td>45.0%</td>
<td>20.00%</td>
<td>$1.13</td>
</tr>
<tr>
<td>2019</td>
<td>Production</td>
<td>0%</td>
<td>67.5%</td>
<td>32.00%</td>
<td>$1.13</td>
</tr>
<tr>
<td>2020</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>19.20%</td>
<td>$1.13</td>
</tr>
<tr>
<td>2021</td>
<td>Production</td>
<td>90.0%</td>
<td>11.52%</td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2022</td>
<td>Production</td>
<td>90.0%</td>
<td>11.52%</td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2023</td>
<td>Production</td>
<td>90.0%</td>
<td>5.76%</td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2024</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2025</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2026</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2027</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2028</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2029</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>2030</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>$1.13</td>
<td></td>
</tr>
<tr>
<td>Year</td>
<td>Description</td>
<td>Percentage</td>
<td>Value</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------</td>
<td>-------------</td>
<td>------------</td>
<td>-------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2031</td>
<td>Production</td>
<td>90.0%</td>
<td>$1.13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2032</td>
<td>Production</td>
<td>90.0%</td>
<td>$1.13</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
10.0 ECONOMIC ANALYSIS

10.1 CASH FLOW ANALYSIS

Table 9.4 shows the profitability, and Table 9.5 shows the cash flow projections for the seventeen-year life of the project assuming a 15% interest rate. The project brings in positive earnings during its first year of production and breaks even during the second year of production. When production is fully scaled up to 90% of the design capacity in the third year of production, the project starts to become extremely profitable, with a cumulative net present value of approximately $263 million.

The internal rate of return of the project is 81.9%, well above the threshold of even the most conservative investors. Additionally, the financials show an ROI of 99.1% in the first year of 90% capacity production. To put these numbers in perspective, Dow Chemical’s stock rose 34.9% in the past five years for an average growth of 6.17% annually.\(^6\) New projects should have higher rates of return than well established companies, and the project IRR and ROI for this project are massive compared to the standard growth in the chemical industry. Overall, the high net present value, internal rate of return, and return on investment all indicate this project will likely be a very profitable endeavor.

<table>
<thead>
<tr>
<th>Table 9.4. Profitability measures</th>
</tr>
</thead>
<tbody>
<tr>
<td>The Internal Rate of Return (IRR) for this project is</td>
</tr>
<tr>
<td>The Net Present Value (NPV) of this project in 2016 is</td>
</tr>
</tbody>
</table>

ROI Analysis (Third Production Year)

| Annual Sales | 204,294,392 |
| Annual Costs | (95,961,647) |
| Depreciation | (4,153,768) |
| Income Tax | (38,546,222) |
| Net Earnings | 65,632,756 |
| Total Capital Investment | 66,243,521 |
| ROI | 99.08% |
Table 9.5. Cash Flow Projections

<table>
<thead>
<tr>
<th>Var Costs</th>
<th>Fixed Costs</th>
<th>Depreciation</th>
<th>Depletion Allowance</th>
<th>Taxable Income</th>
<th>Taxes</th>
<th>Net Earnings</th>
<th>Cash Flow</th>
<th>Cumulative Net Present Value at 15%</th>
</tr>
</thead>
<tbody>
<tr>
<td>(44,202,200)</td>
<td>(7,557,300)</td>
<td>(9,271,800)</td>
<td>-</td>
<td>41,115,900</td>
<td>(15,212,900)</td>
<td>25,903,000</td>
<td>31,594,500</td>
<td>(59,082,800)</td>
</tr>
<tr>
<td>(66,303,200)</td>
<td>(7,557,300)</td>
<td>(14,834,900)</td>
<td>-</td>
<td>64,525,300</td>
<td>(23,874,400)</td>
<td>40,651,000</td>
<td>51,905,500</td>
<td>6,642,300</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>(8,900,900)</td>
<td>-</td>
<td>99,431,800</td>
<td>(36,789,800)</td>
<td>62,642,000</td>
<td>71,543,000</td>
<td>82,461,800</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>(5,340,600)</td>
<td>-</td>
<td>102,992,200</td>
<td>(38,107,100)</td>
<td>64,885,100</td>
<td>70,225,600</td>
<td>138,851,300</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>(2,670,300)</td>
<td>-</td>
<td>105,662,500</td>
<td>(39,095,100)</td>
<td>66,567,400</td>
<td>69,237,600</td>
<td>180,563,000</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>-</td>
<td>-</td>
<td>108,332,700</td>
<td>(40,083,100)</td>
<td>68,249,600</td>
<td>68,249,600</td>
<td>212,103,000</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>-</td>
<td>-</td>
<td>108,332,700</td>
<td>(40,083,100)</td>
<td>68,249,600</td>
<td>68,249,600</td>
<td>235,951,900</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>-</td>
<td>-</td>
<td>108,332,700</td>
<td>(40,083,100)</td>
<td>68,249,600</td>
<td>68,249,600</td>
<td>253,985,000</td>
</tr>
<tr>
<td>(88,404,300)</td>
<td>(7,557,300)</td>
<td>-</td>
<td>-</td>
<td>108,332,700</td>
<td>(40,083,100)</td>
<td>68,249,600</td>
<td>82,571,100</td>
<td>285,360,000</td>
</tr>
</tbody>
</table>
10.2 SENSITIVITY ANALYSIS

Tables 9.6, 9.7, and 9.8 show how the internal rate of return varies from its calculated value as various conditions change. In each chart both condition changes 50% in each direction. Product price was used in each of the charts because that statistic directly leads to either rising or falling revenue and can have a large impact in the IRR for the process. Increasing variable costs would cause the yearly costs to rise. Discrepancies in total permanent investment or fixed costs could come from any issues in this project of sizing or costing different pieces of equipment.

Each of these charts only shows negative internal rates of return in the extreme cases of highly rising costs with a large decrease in revenues from a drop in the price of propylene oxide. This shows how truly safe of an investment this project is. Additionally, any drop in the shown costs or an increase in the price of propylene oxide has the ability to largely increase the IRR of this project.

The main assumptions made in the beginning of the report are that the industrialized process would be able to obtain a selectivity of 99.90% at a conversion of 36.3. This value is based on the 100% selectivity found in laboratory testing. Of the remaining 0.10% that did not yield propylene, 4% reacted to form acetaldehyde, 4% reacted to form acrolein, 4% reacted to form acrylic acid, and 88% reacted to form carbon dioxide. These side product selectivities in themselves were generalized on the knowledge that most of the side product in combustion reactions is in the form of water and carbon dioxide.

<table>
<thead>
<tr>
<th>Selectivity</th>
<th>Water</th>
<th>Acetaldehyde</th>
<th>Acrolein</th>
<th>Acrylic Acid</th>
</tr>
</thead>
<tbody>
<tr>
<td>99.90</td>
<td>3.38E-05</td>
<td>4.56E-05</td>
<td>3.32E-05</td>
<td>3.60E-16</td>
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<tr>
<td>99.89</td>
<td>3.72E-05</td>
<td>5.01E-05</td>
<td>3.65E-05</td>
<td>3.96E-16</td>
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<tr>
<td>99.88</td>
<td>4.06E-05</td>
<td>5.47E-05</td>
<td>3.98E-05</td>
<td>4.32E-16</td>
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<tr>
<td>99.87</td>
<td>4.40E-05</td>
<td>5.93E-05</td>
<td>4.31E-05</td>
<td>4.69E-16</td>
</tr>
<tr>
<td>99.86</td>
<td>4.74E-05</td>
<td>6.38E-05</td>
<td>4.64E-05</td>
<td>5.05E-16</td>
</tr>
<tr>
<td>99.85</td>
<td>5.07E-05</td>
<td>6.84E-05</td>
<td>4.98E-05</td>
<td>5.41E-16</td>
</tr>
<tr>
<td>99.84</td>
<td>5.41E-05</td>
<td>7.30E-05</td>
<td>5.31E-05</td>
<td>5.77E-16</td>
</tr>
<tr>
<td>99.83</td>
<td>5.75E-05</td>
<td>7.75E-05</td>
<td>5.64E-05</td>
<td>6.13E-16</td>
</tr>
<tr>
<td>99.82</td>
<td>6.09E-05</td>
<td>8.21E-05</td>
<td>5.97E-05</td>
<td>6.49E-16</td>
</tr>
<tr>
<td>99.81</td>
<td>6.43E-05</td>
<td>8.67E-05</td>
<td>6.31E-05</td>
<td>6.85E-16</td>
</tr>
<tr>
<td>99.80</td>
<td>6.77E-05</td>
<td>9.12E-05</td>
<td>6.64E-05</td>
<td>7.21E-16</td>
</tr>
<tr>
<td>99.79</td>
<td>7.11E-05</td>
<td>9.58E-05</td>
<td>6.97E-05</td>
<td>7.57E-16</td>
</tr>
<tr>
<td>Spec.</td>
<td>1.00E-04</td>
<td>5.00E-05</td>
<td>2.00E-05</td>
<td></td>
</tr>
</tbody>
</table>

Using these assumptions we found there to be no reason to have a separation unit to separate out acetaldehyde from the process because the 1.15 moles of acetaldehyde fell under the specification of 0.05
wt%. However, Table 9.5a shows that as the design selectivity decreases, the acetaldehyde falls out of specification, specifically at 99.89% selective. The final distillation is responsible for making a separation between acrolein and propylene oxide. Therefore the product contains trace amounts of propylene, trace amounts of acetaldehyde, propylene oxide and acrolein. Because of the relative volatilities shown in Table 9.5b, if the amount of acetaldehyde reaches above 0.005 wt%, another distillation tower would be needed to remove the acetaldehyde from the product stream.

Tables 6.2 – 6.5 show that a change in operating conditions doesn’t change the selectivity very much. All temperatures under 350°C, all times on stream under 30 hours, all pressures at 30 bar or below, and all WHSV at 10,000 or above shows selectivities of 100%. Due to the wide range of operating conditions we believe that the assumption of 99.90% selective is a generous assumption. However, the patent is not detailed enough to make accurate assumptions as to what is a good amount of leeway with possible operating selectivities so there still is a good chance a new distillation column would need to be installed. In addition to the column, the adsorber is designed at a split fraction of 0% of the acetaldehyde being adsorbed. The adsorber is splitting some of the propylene off the process stream so the design assumption that all of the acetaldehyde remains in the process stream may be wrong. If the adsorber would split off some acetaldehyde from the process stream it could result in not needing another distillation tower built for separation of acetaldehyde from the product stream.

<table>
<thead>
<tr>
<th>Table 9.5b. Relative volatilities of process components</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Relative Volatilities</strong></td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
</tr>
<tr>
<td>Propylene</td>
</tr>
<tr>
<td>Acetaldehyde</td>
</tr>
<tr>
<td>PO</td>
</tr>
<tr>
<td>Acrolein</td>
</tr>
<tr>
<td>Water</td>
</tr>
<tr>
<td>Acrylic Acid</td>
</tr>
</tbody>
</table>

If a new tower would need to be installed the reboiler duty would most likely be covered using the steam generated from the reactor. The only additional operating utility costs for a new tower would be the cooling media through the condenser, most likely cooling water, and electricity to run the tower and its components.
**Table 9.6. Sensitivity Analysis for Variable Costs vs. Product Price**

<table>
<thead>
<tr>
<th>Product Price</th>
<th>Variable Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.57</td>
<td>$49,113,511</td>
</tr>
<tr>
<td></td>
<td>$58,936,213</td>
</tr>
<tr>
<td></td>
<td>$68,758,915</td>
</tr>
<tr>
<td></td>
<td>$78,581,617</td>
</tr>
<tr>
<td></td>
<td>$88,404,320</td>
</tr>
<tr>
<td></td>
<td><strong>$98,227,022</strong></td>
</tr>
<tr>
<td>$0.68</td>
<td>$108,049,724</td>
</tr>
<tr>
<td></td>
<td>$117,872,426</td>
</tr>
<tr>
<td></td>
<td>$127,695,128</td>
</tr>
<tr>
<td></td>
<td>$137,517,831</td>
</tr>
<tr>
<td>$1.13</td>
<td>$147,340,533</td>
</tr>
<tr>
<td>$1.36</td>
<td>$156,74%</td>
</tr>
<tr>
<td>$1.59</td>
<td>$152.02%</td>
</tr>
<tr>
<td>$1.70</td>
<td>$156.74%</td>
</tr>
</tbody>
</table>

**Table 9.7. Sensitivity Analysis for Total Permanent Investment vs. Product Price**

<table>
<thead>
<tr>
<th>Product Price</th>
<th>Total Permanent Investment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.57</td>
<td>$25,961,047</td>
</tr>
<tr>
<td></td>
<td>$31,153,256</td>
</tr>
<tr>
<td></td>
<td>$36,345,466</td>
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<tr>
<td></td>
<td>$41,537,675</td>
</tr>
<tr>
<td></td>
<td>$46,729,884</td>
</tr>
<tr>
<td></td>
<td><strong>$51,922,094</strong></td>
</tr>
<tr>
<td>$0.68</td>
<td>$57,114,303</td>
</tr>
<tr>
<td></td>
<td>$62,306,513</td>
</tr>
<tr>
<td></td>
<td>$67,498,722</td>
</tr>
<tr>
<td></td>
<td>$72,690,931</td>
</tr>
<tr>
<td>$1.13</td>
<td>$77,883,141</td>
</tr>
<tr>
<td>$1.36</td>
<td>$223.62%</td>
</tr>
<tr>
<td>$1.59</td>
<td>$258.52%</td>
</tr>
<tr>
<td>$1.70</td>
<td>$302.17%</td>
</tr>
</tbody>
</table>

**Note:** Negative IRR indicates that the investment is not feasible.
Table 9.8. Sensitivity Analysis for Fixed Costs vs. Product Price

<table>
<thead>
<tr>
<th>Product Price</th>
<th>$3,778,664</th>
<th>$4,534,397</th>
<th>$5,290,129</th>
<th>$6,045,862</th>
<th>$6,801,595</th>
<th>$7,557,328</th>
<th>$8,313,060</th>
<th>$9,068,793</th>
<th>$9,824,526</th>
<th>$10,580,259</th>
<th>$11,335,991</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.57</td>
<td>9.76%</td>
<td>8.60%</td>
<td>7.40%</td>
<td>6.16%</td>
<td>4.87%</td>
<td>3.53%</td>
<td>2.12%</td>
<td>0.63%</td>
<td>-0.95%</td>
<td>-2.66%</td>
<td>-4.51%</td>
</tr>
<tr>
<td>$0.68</td>
<td>30.92%</td>
<td>30.11%</td>
<td>29.30%</td>
<td>28.48%</td>
<td>27.67%</td>
<td>26.85%</td>
<td>26.03%</td>
<td>25.20%</td>
<td>24.37%</td>
<td>23.54%</td>
<td>22.70%</td>
</tr>
<tr>
<td>$0.79</td>
<td>46.83%</td>
<td>46.09%</td>
<td>45.35%</td>
<td>44.62%</td>
<td>43.88%</td>
<td>43.15%</td>
<td>42.41%</td>
<td>41.68%</td>
<td>40.94%</td>
<td>40.21%</td>
<td>39.47%</td>
</tr>
<tr>
<td>$0.91</td>
<td>60.74%</td>
<td>60.03%</td>
<td>59.32%</td>
<td>58.62%</td>
<td>57.92%</td>
<td>57.21%</td>
<td>56.51%</td>
<td>55.81%</td>
<td>55.11%</td>
<td>54.41%</td>
<td>53.72%</td>
</tr>
<tr>
<td>$1.02</td>
<td>73.43%</td>
<td>72.75%</td>
<td>72.06%</td>
<td>71.38%</td>
<td>70.69%</td>
<td>70.01%</td>
<td>69.32%</td>
<td>68.64%</td>
<td>67.96%</td>
<td>67.28%</td>
<td>66.61%</td>
</tr>
<tr>
<td><strong>$1.13</strong></td>
<td>85.27%</td>
<td>84.59%</td>
<td>83.92%</td>
<td>83.25%</td>
<td>82.58%</td>
<td>81.91%</td>
<td>81.24%</td>
<td>80.57%</td>
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<td>79.23%</td>
<td>78.57%</td>
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<td>$1.25</td>
<td>96.42%</td>
<td>95.75%</td>
<td>95.09%</td>
<td>94.43%</td>
<td>93.77%</td>
<td>93.11%</td>
<td>92.45%</td>
<td>91.79%</td>
<td>91.14%</td>
<td>90.48%</td>
<td>89.83%</td>
</tr>
<tr>
<td>$1.36</td>
<td>107.01%</td>
<td>106.35%</td>
<td>105.70%</td>
<td>105.05%</td>
<td>104.39%</td>
<td>103.74%</td>
<td>103.09%</td>
<td>102.44%</td>
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<td>$1.47</td>
<td>117.11%</td>
<td>116.47%</td>
<td>115.82%</td>
<td>115.18%</td>
<td>114.54%</td>
<td>113.89%</td>
<td>113.25%</td>
<td>112.61%</td>
<td>111.97%</td>
<td>111.33%</td>
<td>110.69%</td>
</tr>
<tr>
<td>$1.59</td>
<td>126.80%</td>
<td>126.16%</td>
<td>125.53%</td>
<td>124.89%</td>
<td>124.25%</td>
<td>123.62%</td>
<td>122.98%</td>
<td>122.35%</td>
<td>121.72%</td>
<td>121.08%</td>
<td>120.45%</td>
</tr>
<tr>
<td>$1.70</td>
<td>136.11%</td>
<td>135.48%</td>
<td>134.85%</td>
<td>134.22%</td>
<td>133.59%</td>
<td>132.96%</td>
<td>132.34%</td>
<td>131.71%</td>
<td>131.08%</td>
<td>130.46%</td>
<td>129.83%</td>
</tr>
</tbody>
</table>
11.0 OTHER CONSIDERATIONS

11.1 PLANT LOCATION AND LAYOUT

The plant is located in the U.S. Gulf Coast region. Along with a low site factor of 1.00, there are other aspects of the region that make it an attractive area to build this plant. There is a propylene manufacturer on site. As a result, no storage tanks for propylene need to be built. It can simply be taken from the storage tank of the adjacent plant and paid for. Additionally, the gulf coast has an extensive pipeline system containing various gases. Major suppliers such as Air Liquide and Air Products have pipelines transporting oxygen, so oxygen can be taken directly from the pipeline. Plants in other parts of the country have to receive deliveries of oxygen by truck or train. This would necessitate the building of oxygen storage tanks on site and could lead to an unplanned shutdown if oxygen was not delivered on time.

11.2 STARTUP

At plant startup it is necessary to get the reactor up to its operating temperature and pressure before the reaction can begin, so that the catalyst operates at its maximum selectivity and conversion. Additionally, both the propylene and oxygen feed need to come in at their desired molar ratios, temperatures and pressures.

The molar feed ratio issue is of supreme importance. Without the recycle stream, propylene would be entering the reactor at a lower molar ratio, much closer to the dangerous flammable range for a mix of propylene and oxygen. Propylene needs to be released at first at a much higher flowrate. The flowrate in the recycle stream can be monitored, and the flowrate of feed propylene can be reduced gradually as the recycle flowrate increases to its steady-state value.

Additionally, the effluent stream is normally run through heat exchangers E-100 and E-200 to heat up the feed oxygen and propylene streams. Without this effluent stream during startup, the heat exchangers will do nothing to the feed streams. There needs to be a heater on each stream that uses utilities that can heat up the feed streams until the effluent stream reaches its equilibrium temperature and flowrate, so that the heat exchangers will work properly.

11.3 ENVIRONMENTAL CONCERNS AND WATER MANAGEMENT

The reaction proceeds with 99.9% selectivity, producing only a small amount of side products. As a result, only 200 tons of carbon dioxide will be released into the environment per year. Permits can be obtained to release the CO₂, eliminating the need for sequestration.
Although low, carbon dioxide levels will need to be monitored to ensure the plant is following its EPA guidelines. Any additional increase in carbon dioxide production would lead to additional fines and also could be a sign of declining selectivity in the catalyst, meaning that is time to replace it.

Boiler feed water will be heated by the reactor to make 150 lb steam. This steam will then be used to heat the reboilers and then sent back for treatment. The leftover 150 lb steam will be sold as a byproduct of this process.

**11.4 FOULING IN HEAT EXCHANGERS**

Fouling in the heat exchangers that heat the propylene and oxygen feed streams was not accounted for in this design. This fouling could reduce the effective heat transfer coefficient of the heat exchanger, leading to the two streams entering the reactor at too low of a temperature or requiring slightly larger and more expensive heat exchangers. As the two heat exchangers have bare module costs of $181,000 and $40,300 compared to the total bare module cost for the process of $35.7MM, fouling will have a minimal impact on the economics of the process.

**11.4 PROCESS CONTROLLABILITY**

Many control valves and feedback monitors will be needed for this process. Each block needs to be running at its design pressure and temperature to ensure the maximum conversion of propylene to propylene oxide and successful removal of side products. This product quality will be monitored by taking samples of the product stream at regular intervals to detect any unacceptable impurities.

More than any other feedback system, it is crucial that the feed ratio of oxygen to propylene be monitored at all times. Although, the ratio used in this process is well outside of the flammable range, there need to redundant safety systems to cause the plant to shut down if the percentage of oxygen in the reactor starts to rise.
12.0 CONCLUSIONS AND RECOMMENDATIONS

Cutting Costs

One major factor that affects the degree of profitability of this process is the high cost of equipment for the CO$_2$ removal section. Originally a flash drum was selected to flash off the CO$_2$ from the reactor effluent stream but material stream properties made separation difficult. The adsorption-desorption cycle with monoethanolamine (MEA) was used to remove 80% of the CO$_2$ from the stream. Using a size factor scaling estimation, the adsorption cycle was estimated to be a $9,806,000 purchase cost. The CO$_2$ adsorber was recommended by faculty and consultants, as it was necessary for our process workings. However, if alternatives for CO$_2$ removal could be studied for the specific stream composition in the process, the design group believes costs for CO$_2$ removal could be cut significantly, improving the cash position.

The design and profitability analysis for the process to manufacture 200MM lb/year of competitive purity propylene oxide from propylene oxide has been presented. For the prevailing economic conditions, the process has an estimated NPV of $250,133,100 and an IRR of 79.43%. It has also been shown that the process has a positive NPV under various economic scenarios. We recommend conducting research on various ways to reduce costs further.

ASPEN Plus Simulation

During our design of our PO producing plant, the group ran into many Aspen simulation warnings and errors to which were never fully debugged. Many errors in the Aspen calculations were a result of the interactions of carbon dioxide and oxygen gas with the rest of our components (propylene, PO, water, acrolein, acetaldehyde, and acrylic acid). Despite using our engineering intuitions and consultant knowledge to determine that these two gases would act like henry components, Aspen was not able to run simulations without errors. In our final simulations we were able to run the simulation lacking of any errors but we acknowledge that it may not be the most reliable results.

Patent

Many of the assumptions we have made in this design project have been due to insufficient information relating to the patented catalyst technology. The patent for the silver-based catalyst is related to the production of the catalyst and not necessarily a patent for the production of propylene oxide through direct oxidation of propylene. If a design for industrial production of PO was to be invested in, more information and data must be collected from the Council of Scientific and Industrial Research pertaining to the performance and properties of the catalyst.
Reasons for Profitability

One of the biggest reasons for the profitability of this plant design is the high selectivity of the new patented silver-based catalyst. The laboratory results showed 100% selectivity at the operating conditions specified and at other operating conditions similar to the ones chosen for our plant operation. Despite assuming 100% was not possible and choosing a 99.9% selectivity, we still believe that under continuous operation at an industrial capacity plant the selectivity could not be 99.9% for the entirety of operation. Hopefully the 99.9% assumption we made is a generous decrease from the 100% selectivity data set. However, if the selectivity fell below 99.9% the profitability would be very different.

The acetaldehyde specification is 50ppm in the final product and with our current operation at 99.9% selectivity the plant is able to keep all of the acetaldehyde in the product without separation processes and achieve 45ppm of acetaldehyde. This is also assuming that 4% of the unconverted reacted propylene goes to acetaldehyde, a number that was somewhat arbitrarily chosen. There are PO customers that do have specification for their desired product to have a limit of 100ppm of aldehydes which gives the product 99.79% selectivity leeway. If there ends up being too much acetaldehyde in the product, a new separation tower would need to be built that separates the acetaldehyde from the propylene oxide. While this may be a large capital cost, the reboiler utility cost would not be substantial as the steam generated from the reactor would essentially cover the cost for the steam. The new distillation tower would most likely require cooling water which is not a terribly expensive operating cost.

What we believe is the most important measure of a successful product is how consistent our product can be. Not only does the PO have to meet the specifications of the customer but it has to meet the specification on a regular basis. Customers want a product that is reliable and something to which they can be confident about every time they receive a new batch. Therefore, if engineers believe that this can be a reliable and consistent plant design, the industrial use of this catalyst in producing PO has immense upside. Harnessing the heat generated from the highly exothermic reaction via steam generation while producing a pure industrial chemical product both of which have high customer demands, proves the valuable nature of this plant design.

Economics

This project has an NPV of $263MM, an ROI of 99.1%, and an IRR of 81.9%, showing signs of incredible profitability. Additionally, except for the most extreme variations of the price of PO, variable costs, fixed costs, and total permanent investment, the IRR remains strongly positive indicating the high chance of this project’s success even if factors outside of the group’s control negatively affect its economics. Due to its low risk and high reward, a license for the catalyst described in the patent should be acquired, and this process should be developed.
13.0 ACKNOWLEDGEMENTS

We would like to acknowledge and thank the following people for their assistance in our design project:

- Mr. Leonard Fabiano for his instrumental knowledge in process design and for his guidance in solving our many problems with Aspen Plus
- Dr. Rob Riggleman for his suggestions, opinions, and recommendations for the improvement of our industrial process design and in the challenges that we faced
- Our industrial consultant Mr. Bruce Vrana for being a vital resource in the advancement of our design and for offering us his time and guidance
- All of the other industrial consultants that aided in the completion of the design project along with the validity of our designs.

Without the help from all of these professionals, our project could not have been completed thoroughly and well informed. The intentions of all of the professionals were to provide thorough guidance and industry knowledge to which all of the group members are grateful.
14.0 REFERENCES


38. Selective Oxidation of Propylene to Propylene Oxide over Silver-Supported Tungsten Oxide Nanostructure with Molecular Oxygen; Shilpi Ghosh, Shankha S. Acharyya, Ritesh Tiwari, Bipul Sarkar, Rajib K. Singha, Chandrashekar Pendem, Takehiko Sasaki, and Rajaram Bal ACS Catalysis 2014 4 (7), 2169-2174 DOI: 10.1021/cs5004454


APPENDIX A: Aspen Simulation Results

Block Report (Main Process)

BLOCK: A-100    MODEL: SEP

---------------------------
INLET STREAM:          CO2FEED
OUTLET STREAMS:        SEPFEED     CO2OUT
PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

***  MASS AND ENERGY BALANCE ***

IN              OUT        RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)            1202.13         1202.13       -0.189142E-15
MASS(LB/HR   )            57524.0         57524.0        0.126486E-15
ENTHALPY(BTU/HR  )      -0.128436E+08   -0.128715E+08    0.216539E-02

***  CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             63.1981      LB/HR
PRODUCT STREAMS CO2E          63.1981      LB/HR
NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
UTILITIES CO2E PRODUCTION     0.00000      LB/HR
TOTAL CO2E PRODUCTION         0.00000      LB/HR

***  INPUT DATA ***

FLASH SPECS FOR STREAM SEPFEED
TWO    PHASE  TP  FLASH
PRESSURE DROP         PSI                                 0.0
MAXIMUM NO. ITERATIONS                                  150
CONVERGENCE TOLERANCE                                     0.000100000

FLASH SPECS FOR STREAM CO2OUT
TWO    PHASE  TP  FLASH
PRESSURE DROP         PSI                                 0.0
MAXIMUM NO. ITERATIONS                                  150
CONVERGENCE TOLERANCE                                     0.000100000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= CO2OUT    CPT= PROPY-01  FRACTION=          0.100000-05
ACROL-01   0.0
PROPY-02   0.0
OXYGE-01  1.00000
WATER     0.050000
CARBO-01  0.80000
ACETA-01  0.0
ACRYL-01  0.0

*** RESULTS ***

HEAT DUTY             BTU/HR     -27872.
COMPONENT = PROPY-01
STREAM    SUBSTREAM  SPLIT FRACTION
SEPFEED    MIXED      1.00000
CO2OUT     MIXED      0.100000-05
COMPONENT = ACROL-01
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 1.00000

COMPONENT = PROPY-02
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 1.00000

COMPONENT = OXYGE-01
STREAM     SUBSTREAM    SPLIT FRACTION
CO2OUT     MIXED                 1.00000

COMPONENT = WATER
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 0.95000
CO2OUT     MIXED                 0.050000

COMPONENT = CARBO-01
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 0.20000
CO2OUT     MIXED                 0.80000

COMPONENT = ACETA-01
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 1.00000

COMPONENT = ACRYL-01
STREAM     SUBSTREAM    SPLIT FRACTION
SEPFEED    MIXED                 1.00000

BLOCK: DST-100 MODEL: RADFRAC
-------------------------------
INLETS   - SEPFEED STAGE   8
OUTLETS  - DISTVAP1 STAGE   1
            DISTLIQ1 STAGE   1
            BOTTOMS1 STAGE  23
PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***
IN OUT RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)  1200.31 1200.31   -0.189429E-15
MASS(LB/HR)     57452.7 57452.7   0.379927E-15
ENTHALPY(BTU/HR) -0.126730E+08 -0.176444E+08   0.281759

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E     12.6396   LB/HR
PRODUCT STREAMS CO2E  12.6396   LB/HR
NET STREAMS CO2E PRODUCTION  0.00000   LB/HR
UTILITIES CO2E PRODUCTION   1022.65   LB/HR
TOTAL CO2E PRODUCTION     1022.65   LB/HR

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

**** INPUT PARAMETERS ****
NUMBER OF STAGES            23
ALGORITHM OPTION            STANDARD
ABSORBER OPTION         NO
INITIALIZATION OPTION    STANDARD
HYDRAULIC PARAMETER CALCULATIONS NO
INSIDE LOOP CONVERGENCE METHOD BROYDEN
DESIGN SPECIFICATION METHOD NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS 100
MAXIMUM NO. OF INSIDE LOOP ITERATIONS 10
MAXIMUM NUMBER OF FLASH ITERATIONS 150
FLASH TOLERANCE 0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE 0.000100000

**** COL-SPECS ****
MOLAR VAPOR DIST / TOTAL DIST 0.00020000
MOLAR REFUX RATIO 3.56280
DISTILLATE TO FEED RATIO 0.63000

**** PROFILES ****
P-SPEC STAGE 1 PRES, PSIA 246.564

********************

**** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***
OUTLET STREAMS
---------
DISTVAP1 DISTLIQ1 BOTTOMS1

COMPONENT:
PROPY-01 .19993E-03 .99975 .51737E-04
ACROL-01 .35234E-11 .27492E-06 1.0000
PROPY-02 .37414E-07 .77126E-03 .99923
WATER 0.0000 .41714E-12 1.0000
CARBO-01 .52715E-03 .99947 .11599E-06
ACETA-01 .66859E-08 .19512E-03 .99980
ACRYL-01 0.0000 0.0000 1.0000

*** SUMMARY OF KEY RESULTS ***
TOP STAGE TEMPERATURE F 105.756
BOTTOM STAGE TEMPERATURE F 293.154
TOP STAGE LIQUID FLOW LBMOL/HR 1,357.78
BOTTOM STAGE LIQUID FLOW LBMOL/HR 436.440
TOP STAGE VAPOR FLOW LBMOL/HR 0.15277
BOILUP VAPOR FLOW LBMOL/HR 796.161
MOLAR REFUX RATIO 1.77750
MOLAR BOILUP RATIO 1.82422
CONDENSER DUTY (W/O SUBCOOL) BTU/HR -0.116580+08
REBOILER DUTY BTU/HR 6,686,560.

**** MANIPULATED VARIABLES ****

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### MAXIMUM FINAL RELATIVE ERRORS

- DEW POINT: $0.14113 \times 10^{-5}$, STAGE= 13
- BUBBLE POINT: $0.12078 \times 10^{-5}$, STAGE= 13
- COMPONENT MASS BALANCE: $0.20428 \times 10^{-5}$, STAGE= 14, COMP=ACRYL-01
- ENERGY BALANCE: $0.36531 \times 10^{-5}$, STAGE= 13

### PROFILES

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

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### ASSOCIATED UTILITIES
UTILITY USAGE: CW (WATER)
---------------------------------
CONDENSER 1.2989×10^6 2.6076

TOTAL: 1.2989×10^6 LB/HR 2.6076 $/HR

UTILITY USAGE: MPSTEAM (STEAM)
---------------------------------
REBOILER 7643.6516 15.5203 1022.6500

TOTAL: 7643.6516 LB/HR 15.5203 $/HR 1022.6500 CO2 LB/HR

BLOCK: DST-200 MODEL: RADFRAC
---------------------------------
INLETS - SEP2FEED STAGE 7
OUTLETS - PRODUCT STAGE 1
BOTTOMS2 STAGE 14
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

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*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.146613E-05 LB/HR
PRODUCT STREAMS CO2E 0.146613E-05 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 1897.66 LB/HR
TOTAL CO2E PRODUCTION 1897.66 LB/HR

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

**** INPUT PARAMETERS ****

NUMBER OF STAGES 14
ALGORITHM OPTION STANDARD
ABSORBER OPTION NO
INITIALIZATION OPTION STANDARD
HYDRAULIC PARAMETER CALCULATIONS NO
INSIDE LOOP CONVERGENCE METHOD BROYDEN
DESIGN SPECIFICATION METHOD NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS 100
MAXIMUM NO. OF INSIDE LOOP ITERATIONS 10
MAXIMUM NUMBER OF FLASH ITERATIONS 150
FLASH TOLERANCE 0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE 0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST 0.0
MOLAR REFLUX RATIO 2.00000
MOLAR BOTTOMS RATE LBMOL/HR 1.17700

**** PROFILES ****
P-SPEC          STAGE   1  PRES, PSIA                   14.5038

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

*** COMPONENT SPLIT FRACTIONS ***

OUTLET STREAMS

---------------
PRODUCT      BOTTOMS2

COMPONENT:
PROPY-01    1.0000       .51447E-14
ACROL-01    .85737       .14263
PROPY-02    .99982       .18358E-03
WATER       .42132E-01   .95787
CARBO-01    1.0000       0.0000
ACETA-01    1.0000       .16384E-05
ACRYL-01    .72483E-11   1.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE          F                        93.3118
BOTTOM STAGE TEMPERATURE       F                       115.350
TOP STAGE LIQUID FLOW          LBMOL/HR                870.526
BOTTOM STAGE LIQUID FLOW       LBMOL/HR                  1.17700
TOP STAGE VAPOR FLOW           LBMOL/HR                  0.0
BOILUP VAPOR FLOW              LBMOL/HR                987.558
MOLAR REFLUX RATIO             2.00000
MOLAR BOILUP RATIO             839.047
CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                   -0.15292+08
REBOILER DUTY                  BTU/HR                    0.124078+08

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

DEW POINT                       0.13298E-03  STAGE= 14
BUBBLE POINT                    0.85756E-04  STAGE= 14
COMPONENT MASS BALANCE          0.14461E-06  STAGE=  7 COMP=ACRYL-01
ENERGY BALANCE                  0.71322E-05  STAGE= 14

**** PROFILES ****

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

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

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<th>PROPY-02</th>
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### MOLE-Y-PROFILE

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### MASS-X-PROFILE

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*** ASSOCIATED UTILITIES ***

UTILITY USAGE: CW  (WATER)

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<th>Usage</th>
<th>Cost</th>
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<td>Reboiler</td>
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TOTAL: 1.7038E+06 LB/HR  3.4204 $/HR

UTILITY USAGE: LPSTEAM  (STEAM)

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<th>Component</th>
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<tr>
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TOTAL: 1.3167E+04 LB/HR  24.8727 $/HR  1897.6584 CO2 LB/HR

BLOCK: E-100  MODEL: HEATX

THIS BLOCK RUNS WITH ASPEN EDR 34.0 WITH ADVANCED METHOD FOR SHELL&TUBE

HOT SIDE:

INLET STREAM: MIDHEAT
OUTLET STREAM: CO2FEED
PROPERTY OPTION SET: NRTL-RK  RENON (NRTL)/ REDLICH-KWONG
COLD SIDE:
-------------
INLET STREAM: PUMPEDP
OUTLET STREAM: PRXNFEED
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*******************************************************************************
*                                                                        *
*       A POTENTIAL TUBE VIBRATION PROBLEM IS INDICATED                   *
*                                                                        *
*******************************************************************************

*** MASS AND ENERGY BALANCE ***
IN              OUT        RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)            2401.70         2401.70         0.00000
MASS(LB/HR   )            108008.         108008.         0.00000
ENTHALPY(BTU/HR  )       0.639473E+07    0.639473E+07   -0.582556E-15

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             75.8311      LB/HR
PRODUCT STREAMS CO2E          75.8311      LB/HR
NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
UTILITIES CO2E PRODUCTION     0.00000      LB/HR
TOTAL CO2E PRODUCTION         0.00000      LB/HR

*** INPUT DATA ***
FLASH SPECS FOR HOT SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS                                  150
CONVERGENCE TOLERANCE                                     0.000100000

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS                                  150
CONVERGENCE TOLERANCE                                     0.000100000

SHELL&TUBE INPUT FILE NAME                                     \BASE\ROOT\HOMEDIR\FINAL PROJECT PO\E-100.EDR
SHELL&TUBE PROGRAM MODE                                        DESIGN

HEAT CURVE GENERATION
HOT HEAT CURVE GENERATED BY                           ASPEN PLUS
COLD HEAT CURVE GENERATED BY                           ASPEN PLUS

*** OVERALL RESULTS ***
STREAMS:
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<td>P= 4.3279D+02</td>
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<td>V= 1.0000D+00</td>
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<td>V= 1.0000D+00</td>
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UNIT RESULTS:
CALCULATED HEAT DUTY BTU/HR  16094330.4522
CALCULATED (REQUIRED) AREA SQFT  1163.0143
ACTUAL EXCHANGER AREA SQFT  1187.4638
% OVER (UNDER) DESIGN  2.1022
AVERAGE COEFFICIENT BTU/HR-SQFT-R  96.1422
UA BTU/HR-R  111814.7328
LMTD (CORRECTED) F  143.9375
LMTD CORRECTION FACTOR  0.9922
NUMBER OF SHELLS IN SERIES  1
NUMBER OF SHELLS IN PARALLEL  1
HIGH RHOV2 INDICATION NO
VIBRATION INDICATION POSSIBLE

SHELLSIDE RESULTS:
MEAN SHELL METAL TEMPERATURE F  263.3175
TOTAL PRESSURE DROP PSI  3.3878
WINDOW PRESSURE DROP PSI  0.9389
CROSSFLOW PRESSURE DROP PSI  1.6541
BULK FILM COEFFICIENT BTU/HR-SQFT-R  355.5235
WALL FILM COEFFICIENT BTU/HR-SQFT-R  355.5235
THERMAL RESISTANCE HR-SQFT-R/BTU  0.0028
MAXIMUM FOULING RESISTANCE HR-SQFT-R/BTU  0.000109
FOULING RESISTANCE HR-SQFT-R/BTU  0.0000
CROSSFLOW VELOCITY FT/SEC  28.5015
WINDOW VELOCITY FT/SEC  21.1323
MIDPOINT VELOCITY FT/SEC  24.8169
SHELL ENTRANCE RHOV^2 LB/FT-SQSEC  295.8390
SHELL EXIT RHOV^2 LB/FT-SQSEC  1540.8987
BUNDLE ENTRANCE RHOV^2 LB/FT-SQSEC  69.3918
BUNDLE EXIT RHOV^2 LB/FT-SQSEC  1013.3810
FOULING % OF OVERALL RESISTANCE  0.0000
FILM % OF OVERALL RESISTANCE  27.0424
FRICTIONAL PRESSURE DROP PSI  3.3188

TUBESIDE RESULTS:
MEAN TUBE METAL TEMPERATURE F  309.3854
TOTAL PRESSURE DROP PSI  0.6323
BULK FILM COEFFICIENT BTU/HR-SQFT-R  136.9582
WALL FILM COEFFICIENT BTU/HR-SQFT-R  136.9582
THERMAL RESISTANCE HR-SQFT-R/BTU  0.0073
MAXIMUM FOULING RESISTANCE HR-SQFT-R/BTU  0.000109
FOULING RESISTANCE HR-SQFT-R/BTU  0.0000
INPUT VELOCITY FT/SEC  14.9780
OUTLET VELOCITY FT/SEC  3.8149
FOULING % OF OVERALL RESISTANCE  0.0000
FILM % OF OVERALL RESISTANCE  70.1982
FRICTIONAL PRESSURE DROP PSI  0.7039

HEATX COLD-TQCU E-100  TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -3.3878 PSI
PROPERTY OPTION SET: NRTL-RK  RENON (NRTL) / REDLICH-KWONG

! DUTY  ! PRES  ! TEMP  ! VFRAC  !
! ! ! ! !
! ! ! ! !
! ! ! ! !
! ! ! ! !
! BTU/HR  ! PSIA  ! F  !
! ! ! ! !
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HEATX HOT-TQCUR E-100  TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0  PSI
PROPERTY OPTION SET: NRTL-RK  RENON (NRTL) / REDLICH-KWONG
! 9.9632+06 ! 432.7904 ! 327.1361 ! 1.0000 !
!----------------------------------!
! 1.0730+07 ! 432.7904 ! 301.3769 ! 1.0000 !
! 1.1496+07 ! 432.7904 ! 275.8445 ! 1.0000 !
! 1.1953+07 ! 432.7904 ! 260.8642 ! DEW>1.0000 !
! 1.2262+07 ! 432.7904 ! 258.8920 ! 0.9646 !
! 1.3029+07 ! 432.7904 ! 253.7908 ! 0.8750 !
!----------------------------------!
! 1.3497+07 ! 432.7904 ! 250.4973 ! 0.8188 !
! 1.3795+07 ! 432.7904 ! 248.3346 ! 0.7823 !
! 1.4562+07 ! 432.7904 ! 242.5117 ! 0.6852 !
! 1.5328+07 ! 432.7904 ! 236.3098 ! 0.5814 !
! 1.6094+07 ! 432.7904 ! 229.6759 ! 0.4678 !

---

BLOCK: E-200   MODEL: HEATX
---

THIS BLOCK RUNS WITH ASPEN EDR 34.0 WITH ADVANCED METHOD FOR SHELL&TUBE

HOT SIDE:
---

INLET STREAM: RXNOUT
OUTLET STREAM: MIDHEAT
PROPERTY OPTION SET: NRTL-RK  RENON (NRTL) / REDLICH-KWONG

COLD SIDE:
---

INLET STREAM: OXYFEED
OUTLET STREAM: ORXNFEED
PROPERTY OPTION SET: NRTL-RK  RENON (NRTL) / REDLICH-KWONG

***  MASS AND ENERGY BALANCE  ***

IN           OUT        RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR) 1422.13     1422.13      0.00000
MASS(LB/HR)  64563.7    64563.7       0.00000
ENTHALPY(BTU/HR) 0.388772E+07 0.388772E+07 0.00000

***  CO2 EQUIVALENT SUMMARY  ***

FEED STREAMS CO2E  63.1981  LB/HR
PRODUCT STREAMS CO2E  63.1981  LB/HR
NET STREAMS CO2E PRODUCTION  0.00000  LB/HR
UTILITIES CO2E PRODUCTION  0.00000  LB/HR
TOTAL CO2E PRODUCTION  0.00000  LB/HR

***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO PHASE  FLASH
MAXIMUM NO. ITERATIONS  150
CONVERGENCE TOLERANCE  0.000100000

FLASH SPECS FOR COLD SIDE:
TWO PHASE  FLASH
MAXIMUM NO. ITERATIONS  150
CONVERGENCE TOLERANCE  0.000100000

SHELL&TUBE INPUT FILE NAME  \BASE\ROOT\HOMEDIR\FINAL PROJECT PO\E-200.EDR
SHELL&TUBE PROGRAM MODE  DESIGN

HEAT CURVE GENERATION
HOT HEAT CURVE GENERATED BY  ASPEN PLUS
COLD HEAT CURVE GENERATED BY  ASPEN PLUS

---
### **OVERALL RESULTS**

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<tr>
<td>RXNOUT -----</td>
</tr>
<tr>
<td>T= 6.6200D+02</td>
</tr>
<tr>
<td>P= 4.3511D+02</td>
</tr>
<tr>
<td>V= 1.0000D+00</td>
</tr>
</tbody>
</table>

| ORXNFEED | COLD (SHELL) | OXYFEED |
|--------------------------------------|
| T= 4.8200D+02 | T= 7.7000D+01 |
| P= 4.6360D+02 | P= 4.6412D+02 |
| V= 1.0000D+00 | V= 1.0000D+00 |

### UNIT RESULTS:

- **Calculated Heat Duty**: BTU/HR 660800.1009
- **Calculated (Required) Area**: SQFT 34.4999
- **Actual Exchanger Area**: SQFT 55.0699
- **% Over (Under) Design**: 59.6233
- **Average Coefficient**: BTU/HR-SQFT-R 57.0159
- **UA**: BTU/HR-R 1967.0436
- **LMTD (Corrected)**: F 335.9357
- **LMTD Correction Factor**: 0.9974
- **Number of Shells in Series**: 1
- **Number of Shells in Parallel**: 1
- **High RhoV^2 Indication**: NO
- **Vibration Indication**: NO

### Shellside Results:

- **Mean Shell Metal Temperature**: F 311.2545
- **Total Pressure Drop**: PSI 0.5223
- **Window Pressure Drop**: PSI 0.1150
- **Crossflow Pressure Drop**: PSI 0.1541
- **Bulk Film Coefficient**: BTU/HR-SQFT-R 70.2804
- **Wall Film Coefficient**: BTU/HR-SQFT-R 70.2804
- **Thermal Resistance**: HR-SQFT-R/BTU 0.0030
- **Maximum Fouling Resistance**: HR-SQFT-R/BTU 0.005229
- **Fouling Resistance**: HR-SQFT-R/BTU 0.0000
- **Crossflow Velocity**: FT/SEC 18.2846
- **Window Velocity**: FT/SEC 12.3742
- **Midpoint Velocity**: FT/SEC 15.3294
- **Shell Entrance RhoV^2**: LB/FT-SQSEC 147.7776
- **Shell Exit RhoV^2**: LB/FT-SQSEC 266.4837
- **Bundle Entrance RhoV^2**: LB/FT-SQSEC 66.7862
- **Bundle Exit RhoV^2**: LB/FT-SQSEC 120.4338
- **Fouling % of Overall Resistance**: 0.0000
- **Film % of Overall Resistance**: 81.1263
- **Frictional Pressure Drop**: PSI 0.5174

### Tubeside Results:

- **Mean Tube Metal Temperature**: F 593.1859
- **Total Pressure Drop**: PSI 2.3228
- **Bulk Film Coefficient**: BTU/HR-SQFT-R 333.5018
- **Wall Film Coefficient**: BTU/HR-SQFT-R 333.5018
- **Thermal Resistance**: HR-SQFT-R/BTU 0.0030
- **Maximum Fouling Resistance**: HR-SQFT-R/BTU 0.005229
- **Fouling Resistance**: HR-SQFT-R/BTU 0.0000
- **Input Velocity**: FT/SEC 62.4803
- **Outlet Velocity**: FT/SEC 61.5096
- **Fouling % of Overall Resistance**: 0.0000
# HEATX COLD-TQCU E-200  TQCURV INLET

**PRESSURE PROFILE:** CONSTANT2  
**PRESSURE DROP:** -0.5223 PSI  
**PROPERTY OPTION SET:** NRTL-RK  

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<th>VFRAC</th>
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</table>

# HEATX HOT-TQCUR E-200  TQCURV INLET

**PRESSURE PROFILE:** CONSTANT2  
**PRESSURE DROP:** 0.0 PSI  
**PROPERTY OPTION SET:** NRTL-RK  

<table>
<thead>
<tr>
<th>DUTY</th>
<th>PRES</th>
<th>TEMP</th>
<th>VFRAC</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
<td>6.2933+04</td>
<td>435.1132</td>
<td>660.1721</td>
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<td>INLET STREAMS:</td>
<td>OUTLET STREAM:</td>
<td>PROPERTY OPTION SET:</td>
</tr>
<tr>
<td>---------------</td>
<td>----------------</td>
<td>----------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>TOTAL BALANCE</td>
<td>MOLE(LBMOL/HR)</td>
<td>1199.56</td>
<td>NRTL-RK RENON (NRTL) / REDLICH-KWONG</td>
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<tr>
<td></td>
<td>MASS(LB/HR)</td>
<td>50484.3</td>
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</tr>
<tr>
<td></td>
<td>ENTHALPY(BTU/HR)</td>
<td>0.303729E+07</td>
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</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

| FEED STREAMS CO2E | 12.6330 | LB/HR |
| PRODUCT STREAMS CO2E | 12.6330 | LB/HR |
| NET STREAMS CO2E PRODUCTION | 0.121916E-07 | LB/HR |
| UTILITIES CO2E PRODUCTION | 0.0000 | LB/HR |
| TOTAL CO2E PRODUCTION | 0.121916E-07 | LB/HR |

*** INPUT DATA ***

| TWO PHASE | FLASH |
| MAXIMUM NO. ITERATIONS | 150 |
| CONVERGENCE TOLERANCE | 0.000100000 |
| OUTLET PRESSURE | MINIMUM OF INLET STREAM PRESSURES |

BLOCK: M-2  MODEL: MIXER

INLET STREAMS: PRXNFEED ORXNFEED
OUTLET STREAM: RXNFEED
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

| TOTAL BALANCE | MOLE(LBMOL/HR) | 1419.56        | NRTL-RK RENON (NRTL) / REDLICH-KWONG |
|               | MASS(LB/HR)    | 57524.0        |                       |
|               | ENTHALPY(BTU/HR) | 0.889217E-06  |                       |
###ENTHALPY (BTU/HR)
|          | 0.198753E+08 | 0.198753E+08 | 0.895473E-06 |

###CO2 EQUIVALENT SUMMARY***
- **FEED STREAMS CO2E**: 12.6330 LB/HR
- **PRODUCT STREAMS CO2E**: 12.6323 LB/HR
- **NET STREAMS CO2E PRODUCTION**: -0.643809E-03 LB/HR
- **UTILITIES CO2E PRODUCTION**: 0.00000 LB/HR
- **TOTAL CO2E PRODUCTION**: -0.643809E-03 LB/HR

###INPUT DATA***
- **TWO PHASE FLASH**
- **MAXIMUM NO. ITERATIONS**: 150
- **CONVERGENCE TOLERANCE**: 0.000100000
- **OUTLET PRESSURE**: MINIMUM OF INLET STREAM PRESURES

**BLOCK**: P-1  **MODEL**: PUMP

-------------

**INLET STREAM**: MIXED
**OUTLET STREAM**: PUMPEDP
**PROPERTY OPTION SET**: NRTL-RK RENON (NRTL) / REDLICH-KWONG

###MASS AND ENERGY BALANCE***

<table>
<thead>
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<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
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<tr>
<td><strong>MOLE (LB/HR)</strong></td>
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<td><strong>ENTHALPY (BTU/HR)</strong></td>
<td>0.303729E+07</td>
<td>0.314401E+07</td>
<td>-0.339435E-01</td>
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</table>

###CO2 EQUIVALENT SUMMARY***
- **FEED STREAMS CO2E**: 12.6330 LB/HR
- **PRODUCT STREAMS CO2E**: 12.6330 LB/HR
- **NET STREAMS CO2E PRODUCTION**: 0.00000 LB/HR
- **UTILITIES CO2E PRODUCTION**: 0.00000 LB/HR
- **TOTAL CO2E PRODUCTION**: 0.00000 LB/HR

###INPUT DATA***
- **OUTLET PRESSURE** PSIA: 464.121
- **DRIVER EFFICIENCY**: 1.00000

**FLASH SPECIFICATIONS**:  
- **LIQUID PHASE CALCULATION**: NO FLASH PERFORMED  
- **MAXIMUM NUMBER OF ITERATIONS**: 150  
- **TOLERANCE**: 0.000100000

###RESULTS***
- **VOLUMETRIC FLOW RATE** CUFT/HR: 1,651.06  
- **PRESSURE CHANGE** PSI: 217.557  
- **NPSH AVAILABLE** FT-LBF/LB: 139.412  
- **FLUID POWER** HP: 26.1235  
- **BRAKE POWER** HP: 41.9420  
- **ELECTRICITY KW**: 31.2761  
- **PUMP EFFICIENCY USED**: 0.62285  
- **NET WORK REQUIRED** HP: 41.9420  
- **HEAD DEVELOPED FT-LBF/LB**: 1,024.57

**BLOCK**: R-100  **MODEL**: RSTOIC

-------------

**INLET STREAM**: RXNFEED  
**OUTLET STREAM**: RXNOUT  
**PROPERTY OPTION SET**: NRTL-RK RENON (NRTL) / REDLICH-KWONG
*** MASS AND ENERGY BALANCE ***

IN        OUT       GENERATION   RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)         1419.56       1202.13      -217.429      0.160172E-15
MASS(LB/HR)           57524.0       57524.0                   -0.126486E-15
ENTHALPY(BTU/HR)    0.198753E+08  0.391152E+07                0.803197

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             12.6323      LB/HR
PRODUCT STREAMS CO2E          63.1981      LB/HR
NET STREAMS CO2E PRODUCTION   50.5658      LB/HR
UTILITIES CO2E PRODUCTION     0.00000      LB/HR
TOTAL CO2E PRODUCTION         50.5658      LB/HR

*** INPUT DATA ***
STOICHIOMETRY MATRIX:

REACTION # 1:
SUBSTREAM MIXED :
PROPY-01 -1.00    PROPY-02 1.00    OXYGE-01 -0.500

REACTION # 2:
SUBSTREAM MIXED :
PROPY-01 -2.00    OXYGE-01 -9.00    WATER 6.00    CARBO-01 6.00

REACTION # 3:
SUBSTREAM MIXED :
PROPY-01 -2.00    OXYGE-01 -1.50    ACETA-01 3.00

REACTION # 4:
SUBSTREAM MIXED :
PROPY-01 -1.00    ACROL-01 1.00    OXYGE-01 -1.00    WATER 1.00

REACTION # 5:
SUBSTREAM MIXED :
PROPY-01 -1.00    OXYGE-01 -1.50    WATER 1.00    ACRYL-01 1.00

REACTION CONVERSION SPECS: NUMBER=    5
REACTION # 1:
SUBSTREAM:MIXED KEY COMP:PROPY-01 CONV FRAC: 0.3630
REACTION # 2:
SUBSTREAM:MIXED KEY COMP:PROPY-01 CONV FRAC: 0.3194E-03
REACTION # 3:
SUBSTREAM:MIXED KEY COMP:PROPY-01 CONV FRAC: 0.1452E-04
REACTION # 4:
SUBSTREAM:MIXED KEY COMP:PROPY-01 CONV FRAC: 0.1452E-04
REACTION # 5:
SUBSTREAM:MIXED KEY COMP:PROPY-01 CONV FRAC: 0.1452E-04

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE F                                 662.000
SPECIFIED PRESSURE    PSIA                              435.113
MAXIMUM NO. ITERATIONS                                  150
CONVERGENCE TOLERANCE                                     0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

*** RESULTS ***
OUTLET TEMPERATURE    F                                    662.00
OUTLET PRESSURE       PSIA                                 435.11
HEAT DUTY             BTU/HR                             -0.15948E+08
VAPOR FRACTION                                             1.0000

REACTION EXTENTS:

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<th>REACTION NUMBER</th>
<th>REACTION EXTENT</th>
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<td>LBMOL/HR</td>
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<tr>
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V-L PHASE EQUILIBRIUM:

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<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
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DYNAMICS

DYNAMICS RESULTS=ON

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES FLASH-MAXIT=150

MODEL-OPTION

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DATABASES 'APV88 PURE32'/ 'APV88 AQUEOUS'/ 'APV88 SOLIDS'/ &
'APV88 INORGANIC'/ 'APEOSV88 AP-EOS'/ 'NOASPENPCD'
PROP-SOURCES 'APV88 PURE32' / 'APV88 AQUEOUS' / 'APV88 SOLIDS' & / 'APV88 INORGANIC' / 'APEOSV88 AP-EOS'

COMPONENTS
  PROPY-01 C3H6-2 /
  ACROL-01 C3H4O /
  PROPY-02 C3H6O-4 /
  OXYGE-01 O2 /
  WATER H2O /
  CARBO-01 CO2 /
  ACETA-01 C2H4O-1 /
  ACRYL-01 C3H4O2-1

HENRY-COMPS HC-1 OXYGE-01 CARBO-01

SOLVE
  RUN-MODE MODE=SIM

FLOWSHEET
  BLOCK P-1 IN=MIXED OUT=PUMPEDP
  BLOCK E-100 IN=MIDHEAT PUMPEDP OUT=CO2FEED PRXNFEED
  BLOCK E-200 IN=RXNOUT OXYFEED OUT=MIDHEAT ORXNFEED
  BLOCK R-100 IN=RXNFEED OUT=RXNOUT
  BLOCK DST-200 IN=SEP2FEED OUT=PRODUCT BOTTOMS2
  BLOCK VALVE IN=BOTTOMS1 OUT=SEP2FEED
  BLOCK A-100 IN=CO2FEED OUT=SEPFEED CO2OUT
  BLOCK M-2 IN=PRXNFEED ORXNFEED OUT=RXNFEED
  BLOCK M-1 IN=PROPFEED RECYCLE OUT=MIXED
  BLOCK DST-100 IN=SEPFEED OUT=DISTVAP1 DISTLIQ1 BOTTOMS1

PROPERTIES NRTL-RK
  PROPERTIES OLI

PROP-DATA HENRY-1
  IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar &
  INVERSE-PRES=’1/bar’
  PROP-LIST HENRY
  BPVAL OXYGE-01 WATER 144.4080745 -7775.060000 -18.39740000 &
  -.94435400E-3 .8500000000 74.85000000 0.0
  BPVAL CARBO-01 WATER 159.1996745 -8477.711000 -21.95743000 &
  5.78074800E-3 -.1500000000 226.8500000 0.0
  BPVAL PROPY-01 PROPY-02 0.0 244.2667000 .3000000000 0.0 &
  0.0 0.0 25.00000000 30.05000000
  BPVAL PROPY-02 PROPY-01 0.0 -8.806400000 .3000000000 0.0 &
  0.0 0.0 25.00000000 30.05000000
  BPVAL ACROL-01 WATER 0.0 588.5895000 .4400000000 0.0 0.0 &
  0.0 18.35000000 92.10000000
  BPVAL WATER ACROL-01 0.0 749.9613000 .4400000000 0.0 0.0 &
  0.0 18.35000000 92.10000000
  BPVAL PROPY-02 WATER 0.0 303.5255000 .3000000000 0.0 0.0 &
  0.0 34.90000000 99.00000000
BPVAL WATER PROPY-02 0.0 686.0125000 .3000000000 0.0 0.0 0.0 0.0 34.90000000 99.00000000
BPVAL PROPY-02 ACETA-01 0.0 -41.98650000 .3000000000 0.0 0.0 0.0 0.0 20.25000000 34.25000000
BPVAL ACETA-01 PROPY-02 0.0 76.57290000 .3000000000 0.0 0.0 0.0 0.0 20.25000000 34.25000000
BPVAL WATER CARBO-01 10.06400000 -3268.135000 .2000000000 0.0 0.0 0.0 0.0 200.0000000
BPVAL CARBO-01 WATER 10.06400000 -3268.135000 .2000000000 0.0 0.0 0.0 0.0 200.0000000
BPVAL WATER ACETA-01 -1.132900000 569.7382000 .3000000000 0.0 0.0 0.0 0.0 10.00000000 75.00000000
BPVAL ACETA-01 WATER 17.10250000 -4681.343300 .3000000000 0.0 0.0 0.0 0.0 100.4000000 120.5000000
BPVAL WATER ACRYL-01 0.0 924.2531000 .3000000000 0.0 0.0 0.0 0.0 100.4000000 120.5000000
BPVAL ACRYL-01 WATER 0.0 -300.0066000 .3000000000 0.0 0.0 0.0 0.0 100.4000000 120.5000000

STREAM OXYFEED
   SUBSTREAM MIXED TEMP=77.00000000 PRES=464.1207607
   MOLE-FLOW OXYGE-01 220.0000000

STREAM PROPFEED
   SUBSTREAM MIXED TEMP=77.00000000 PRES=246.5641541
   MOLE-FLOW PROPY-01 1198.940000

BLOCK M-1 MIXER
   PARAM

BLOCK M-2 MIXER
   PARAM

BLOCK A-100 SEP
   PARAM
   FRAC STREAM=CO2OUT SUBSTREAM=MIXED COMPS=PROPY-01 ACROL-01 & PROPY-02 OXYGE-01 WATER CARBO-01 ACETA-01 ACRYL-01 & FRACS=1E-006 0. 0. 1. 0.05 0.8 0. 0.

BLOCK E-100 HEATX
   PARAM T-COLD=250. <C> CALC-TYPE=DESIGN & CALC-METHOD=TASCIPLUS-RIG
   HETRAN-PARAM INPUT-FILE= & '\base\root\hommedir\Final Project PO\E-100.edr'
   FEEDS HOT=MIDHEAT COLD=PUMPEDP
   OUTLETS-HOT CO2FEED
   OUTLETS-COLD PRXNFEED
   HOT-SIDE SHELL-TUBE=TUBE DP-OPTION=CONSTANT DPPARMOPT=NO
   COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
   TQ-PARAM CURVE=YES

BLOCK E-200 HEATX
   PARAM T-COLD=250. <C> CALC-TYPE=DESIGN & CALC-METHOD=TASCIPLUS-RIG
   HETRAN-PARAM INPUT-FILE= & '\base\root\hommedir\Final Project PO\E-200.edr'
FEEDS HOT=RXNOUT COLD=OXYFEED
OUTLETS-HOT MIDHEAT
OUTLETS-COLD ORXNFEED
HOT-SIDE SHELL-TUBE=TUBE DP-OPTION=CONSTANT DPPARMOPT=NO
COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
TQ-PARAM CURVE=YES

BLOCK DST-100 RADFRAC
PARAM NSTAGE=23 ALGORITHM=STANDARD MAXOL=100 DAMPING=NONE
COL-CONFIG CONDENSER=PARTIAL-V-L
FEEDS SEPFEED 8
PRODUCTS DISTLIQ1 1 L / BOTTOMS1 23 L / DISTVAP1 1 V
P-SPEC 1 246.5641541
COL-SPECS D:F=0.63 MOLE-RDV=0.0002 MOLE-RR=3.5628
SPEC 1 MASS-FRAC 0.999 COMPS=PROP-01 STREAMS=DISTLIQ1 &
   SPEC-DESCRIP="Purity"
SPEC 2 MASS-FRAC 0.999 COMPS=PROP-02 STREAMS=BOTTOMS1 &
   SPEC-DESCRIP="PurityB"
VARY 1 MOLE-RR 1. 10.
VARY 2 D:F 0.2 0.9
UTILITIES COND-UTIL=CW REB-UTIL=MPSTEAM

BLOCK DST-200 RADFRAC
PARAM NSTAGE=14 ALGORITHM=STANDARD MAXOL=100 DAMPING=NONE
COL-CONFIG CONDENSER=TOTAL
FEEDS SEP2FEED 7
PRODUCTS PRODUCT 1 L / BOTTOMS2 14 L
P-SPEC 1 14.50377377
COL-SPECS MOLE-B=1.177000000 MOLE-RR=2.
UTILITIES COND-UTIL=CW REB-UTIL=LPSTEAM

BLOCK R-100 RSTOIC
PARAM TEMP=662.0000000 PRES=435.1132132
STOIC 1 MIXED PROP-01 -1. / OXYGE-01 -0.5 / PROP-02 &
   1.
STOIC 2 MIXED PROP-01 -2. / OXYGE-01 -9. / CARBO-01 6. / &
   WATER 6.
STOIC 3 MIXED PROP-01 -2. / OXYGE-01 -1.5 / ACETA-01 &
   3.
STOIC 4 MIXED PROP-01 -1. / OXYGE-01 -1. / ACROL-01 1. / &
   WATER 1.
STOIC 5 MIXED PROP-01 -1. / OXYGE-01 -1.5 / ACRYL-01 &
   1. / WATER 1.
CONV 1 MIXED PROP-01 0.363
CONV 2 MIXED PROP-01 0.00031944
CONV 3 MIXED PROP-01 1.452E-005
CONV 4 MIXED PROP-01 1.452E-005
CONV 5 MIXED PROP-01 1.452E-005

BLOCK P-1 PUMP
PARAM PRES=464.1207607

BLOCK VALVE VALVE
PARAM P-OUT=14.50377377

STREAM-PRICE
STREAM-PRICE STREAM=OXYFEED MASS-PRICE=.091000000 / &
STREAM=PRODUCT MASS-PRICE=1.134000000 / STREAM=PROPFEED &
MASS-PRICE=.499000000

UTILITY CW GENERAL
DESCRIPTION "Cooling Water, Inlet Temp=20 C, Outlet Temp=25 C"
COST ENERGY-PRICE=2.23671841E-7
PARAM UTILITY-TYPE=WATER PRES=14.69594878 &
PRES-OUT=14.69594878 TIN=68.00000000 TOUT=77.00000000 &
CALOPT=FLASH MIN-TAPP=9.00000000 HTC=660.4131888

UTILITY LPSTEAM GENERAL
DESCRIPTION &
"Low Pressure Steam, Inlet Temp=125 C, Outlet Temp=124 C"
COST ENERGY-PRICE=2.00460612E-6
PARAM UTILITY-TYPE=STEAM TIN=257.0000000 TOUT=255.2000000 &
VFRAC=1. VFR-OUT=0. CALOPT=FLASH MIN-TAPP=18.00000000 &
CALCCO2=YES FACTORSOURCE="US-EPA-Rule-E9-5711" FUELSOURCE= &
"Natural_gas" CO2FACTOR=1.30000000E-4 EFFICIENCY=0.85 &
HTC=1056.661102

UTILITY MPSTEAM GENERAL
DESCRIPTION &
"Medium Pressure Steam, Inlet Temp=175 C, Outlet Temp=174 C, Pres=127 psia"
COST ENERGY-PRICE=2.32112288E-6
PARAM UTILITY-TYPE=STEAM TIN=347.0000000 TOUT=345.2000000 &
VFRAC=1. VFR-OUT=0. CALOPT=FLASH MIN-TAPP=18.00000000 &
CALCCO2=YES FACTORSOURCE="US-EPA-Rule-E9-5711" FUELSOURCE= &
"Natural_gas" CO2FACTOR=1.30000000E-4 EFFICIENCY=0.85 &
HTC=1056.661102

DESIGN-SPEC DS-1
DEFINE P MOLE-FLOW STREAM=MIXED SUBSTREAM=MIXED &
COMPONENT=PROPY-01 UOM="lbmol/hr"
SPEC "p" TO "1198.94"
TOL-SPEC ".5"
VARY MOLE-FLOW STREAM=PROPFEED SUBSTREAM=MIXED &
COMPONENT=PROPY-01 UOM="lbmol/hr"
LIMITS "0" "1200"

DESIGN-SPEC DS-2
DEFINE O MOLE-FLOW STREAM=RXNFEED SUBSTREAM=MIXED &
COMPONENT=OXYGE-01 UOM="lbmol/hr"
SPEC "o" TO "220"
TOL-SPEC ".5"
VARY MOLE-FLOW STREAM=OXYFEED SUBSTREAM=MIXED &
COMPONENT=OXYGE-01 UOM="lbmol/hr"
LIMITS "0" "240"

EO-CONV-OPTI
TRANSFER T-1
SET STREAM RECYCLE
EQUAL-TO STREAM DISTLIQ1

STREAM-REPOR MOLEFLOW MASSFLOW MASSFRAC
Block Report (Steam Generation)

BLOCK: F-100   MODEL: FLASH2

INLET STREAM: WATERIN
OUTLET VAPOR STREAM: 150STEAM
OUTLET LIQUID STREAM: LIQUID
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>6125.97</td>
<td>6125.97</td>
<td>0.00000</td>
</tr>
<tr>
<td>MASS(LB/HR)</td>
<td>110361.</td>
<td>110361.</td>
<td>0.00000</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.719236E+09</td>
<td>-0.624029E+09</td>
<td>-0.132372</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION 0.00000 LB/HR

*** INPUT DATA ***

TWO PHASE TV FLASH
SPECIFIED TEMPERATURE F 358.438
VAPOR FRACTION 1.0000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.0001

*** RESULTS ***

OUTLET TEMPERATURE F 358.44
OUTLET PRESSURE PSIA 149.69
HEAT DUTY BTU/HR 95207E+08
VAPOR FRACTION 1.0000

V-L PHASE EQUILIBRIUM:

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

BLOCK: P-3   MODEL: PUMP

INLET STREAM: BFWATRIN
OUTLET STREAM: WATERIN
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

126
TOTAL BALANCE
MOLE(LBMOL/HR)  6125.97   6125.97  0.00000
MASS(LB/HR ) 110361. 110361. 0.00000
ENTHALPY(BTU/HR ) -0.719333E+09  -0.719236E+09  -0.134888E-03

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E  0.00000  LB/HR
PRODUCT STREAMS CO2E  0.00000  LB/HR
NET STREAMS CO2E PRODUCTION  0.00000  LB/HR
UTILITIES CO2E PRODUCTION  0.00000  LB/HR
TOTAL CO2E PRODUCTION  0.00000  LB/HR

*** INPUT DATA ***
OUTLET PRESSURE  PSIA  174.045
DRIVER EFFICIENCY  1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION
NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS  30
TOLERANCE  0.000100000

*** RESULTS ***
VOLUMETRIC FLOW RATE  CUFT/HR  2,140.24
PRESSURE CHANGE  PSI  159.542
NPSH AVAILABLE  FT-LBF/LB  -377.526
FLUID POWER  HP  24.8332
BRAKE POWER  HP  38.1341
ELECTRICITY  KW  28.4366
PUMP EFFICIENCY USED  0.65121
NET WORK REQUIRED  HP  38.1341
HEAD DEVELOPED  FT-LBF/LB  445.535
NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.

Block Report (Recycle Pump)

BLOCK:  P-2  MODEL: PUMP
----------
INLET STREAM: DISTLIQ1
OUTLET STREAM:  2
PROPERTY OPTION SET:  NRTL-RK  RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***
IN   OUT   RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)  763.719  763.719  0.00000
MASS(LB/HR ) 32143.7  32143.7  0.00000
ENTHALPY(BTU/HR ) 0.214718E+07  0.215221E+07  -0.234153E-02

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E  12.6330  LB/HR
PRODUCT STREAMS CO2E  12.6330  LB/HR
NET STREAMS CO2E PRODUCTION  0.00000  LB/HR
UTILITIES CO2E PRODUCTION  1.12954  LB/HR
TOTAL CO2E PRODUCTION  1.12954  LB/HR
*** INPUT DATA ***
OUTLET PRESSURE  PSIA 261.068
DRIVER EFFICIENCY 1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION
NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS 30
TOLERANCE 0.000100000

*** RESULTS ***
VOLUMETRIC FLOW RATE  CUFT/HR 1,074.75
PRESSURE CHANGE  PSI 14.5038
NPSH AVAILABLE  FT-LBF/LB 0.40638
FLUID POWER  HP 1.13366
BRAKE POWER  HP 1.98059
ELECTRICITY  KW 1.47693
PUMP EFFICIENCY USED 0.57239
NET WORK REQUIRED  HP 1.98059
HEAD DEVELOPED FT-LBF/LB 69.8318

*** ASSOCIATED UTILITIES ***
UTILITY ID FOR ELECTRICITY U-1
RATE OF CONSUMPTION 1.4769  KW
COST 7.7243-02 $/HR
CO2 EQUIVALENT EMISSIONS 1.1295 LB/HR
APPENDIX B: Sample Calculations

Boiler Feedwater

\[ Q(0.99) = \dot{m}[H_{181^\circ C} - H_{100^\circ C}] \]

\[ \frac{(0.99)(4,957,297)}{772.1 - 419.9} = \dot{m} = 13,267.71 \frac{g}{s} \text{ of boiler feedwater} \]

\[ 13,267.71 \frac{g}{s} = 110,361.09 \frac{lb}{hr} \]

\[ \frac{110,361.09 \frac{lb}{hr}}{8.33} = 13,248.63 \frac{gal}{hr} \]

Steam Needed

\[ RB_1 = 1,964,420 \ W \]

\[ RB_2 = 3,636,540 \ W \]

\[ Q = \dot{m}[H_{\text{steam,181^\circ C}} - H_{\text{water,181^\circ C}}] \]

\[ \frac{5,600,960}{[2782.23 - 772.1]} = \dot{m} = 2786.37 \frac{g}{s} \]

\[ \dot{m} = 2786.37 \frac{g}{s} = 22,068.03 \frac{lb}{hr} \text{ of 150lb steam used in reboilers} \]

Cooling Water

\[ Q_{\text{cond}} = \dot{m}H \]

\[ 3,415,870 = Q_{\text{DST-100}} = \dot{m}[127.29] \]

\[ \dot{m} = 26,835.34 \frac{g}{s} = 212,535.87 \frac{lb}{hr} \]

\[ 212,535.87 \frac{lb}{hr} = 25,597.48 \frac{gal}{hr} \text{ for condenser CD-1} \]

Adsorber Costing
\[
\left( \frac{\text{Flow Rate of Source}}{	ext{Our Flow Rate}} \right)^{0.9} = \left( \frac{\text{Price of Source}}{\text{Our Price}} \right) = \left( \frac{9.45 \times 10^6 \frac{\text{lb}}{\text{hr}}}{57,491.34 \frac{\text{lb}}{\text{hr}}} \right)^{0.9} = 98.64
\]

\[\text{Our Price} = \frac{967,315,790}{98.68} = 9,806,000\]

Reactor Sizing
\[Q = UA\Delta T_{LM}\]
\[\Delta T_1 = 4133 - 454\]
\[\Delta T_2 = 623 - 373\]
\[\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{\ln \left(\frac{\Delta T_1}{\Delta T_2}\right)} = 1275.23\]
\[U = 300 \frac{W}{m^2\text{C}} \text{ (assumed, high pressure pas in tubes, liq on shell side)}\]
\[A = \frac{4,678,000}{(300)(1275.23)} = 12.23 \text{ m}^2\]
\[N_t = \frac{A_i}{A_tN_p} = \frac{A_i}{A_t} = \frac{131.34 \text{ ft}^2}{\pi \left(\frac{0.75}{12} \text{ ft}\right) (8 \text{ ft})} = 83.80 \text{ 3/4" tubes}\]

Reactor Costing
\[C_{\text{purchase}} = F_pF_MF_LC_B\]
\[C_B = \exp(11.147 - .9186\ln(A) + 0.09790(\ln(A))^2) = 8,067.44\]
\[F_M = 1.75 + \left(\frac{A}{100}\right)^{0.13} = 2.79\]
\[F_p = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017\left(\frac{P}{100}\right)^2 = 1.017\]
\[F_L = 1.25 \text{ for 8' length}\]
\[C_{\text{purchase}} = F_pF_MF_LC_B = $28,606.94\]
# APPENDIX C: Material Safety Data Sheets

## SAFETY DATA SHEET

### Propylene

### Section 1. Identification

<table>
<thead>
<tr>
<th>GHS product identifier</th>
<th>Propylene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical name</td>
<td>propylene</td>
</tr>
<tr>
<td>Other means of identification</td>
<td>Propene, methylethene, methylethylene, 1-propene, 1-propylene, refrigerant gas R1270</td>
</tr>
<tr>
<td>Product use</td>
<td>Synthetic/Analytical chemistry.</td>
</tr>
<tr>
<td>Synonym</td>
<td>Propene, methylethene, methylethylene, 1-propene, 1-propylene, refrigerant gas R1270</td>
</tr>
<tr>
<td>SDS #</td>
<td>001046</td>
</tr>
</tbody>
</table>
| Supplier's details     | Airgas USA, LLC and its affiliates  
259 North Radnor-Chester Road  
Suite 100  
Radnor, PA 19087-5283  
1-810-687-5253 |
| Emergency telephone number (with hours of operation) | 1-888-734-3438 |

### Section 2. Hazards identification

<table>
<thead>
<tr>
<th>OSHA/HCS status</th>
<th>This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).</th>
</tr>
</thead>
</table>
| Classification of the substance or mixture | FLAMMABLE GASES - Category 1  
GASES UNDER PRESSURE - Liquefied gas |
| GHS label elements | Hazard pictograms: ![Flammable](image) ![Explosion](image) |
| Signal word | Danger |
| Hazard statements | Extremely flammable gas.  
Contains gas under pressure; may explode if heated.  
May cause frostbite.  
May form explosive mixtures in Air.  
May displace oxygen and cause rapid suffocation. |
| Precautionary statements | General: Read and follow all Safety Data Sheets (SDS’S) before use. Read label before use.  
Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use.  
Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction. Always keep container in upright position. Approach suspected leak area with caution.  
Prevention: Never Put cylinders into unventilated areas of passenger vehicles. Keep away from heat, sparks, open flames and hot surfaces. - No smoking. Use and store only outdoors or in a well ventilated place.  
Response: Leaking gas fire: Do not extinguish, unless leak can be stopped safely. Eliminate all ignition sources if safe to do so. |

| Date of issue/Date of revision | 7/27/2015.  
Date of previous issue | 10/16/2014.  
Version | 0.04 | 1/12 |
Section 2. Hazards identification

Storage: Protect from sunlight. Protect from sunlight when ambient temperature exceeds 52°C/125°F. Store in a well-ventilated place.

Disposal: Not applicable.

Hazards not otherwise classified: In addition to any other important health or physical hazards, this product may displace oxygen and cause rapid suffocation.

Section 3. Composition/information on ingredients

Substance/mixture: Substance

Chemical name: propylene

Other means of identification: Propene, methylethane, methylethylene, 1-propene, 1-propylene, refrigerant gas

R1270

CAS number/other identifiers

CAS number: 115-07-1

Product code: 001046

<table>
<thead>
<tr>
<th>Ingredient name</th>
<th>%</th>
<th>CAS number</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene</td>
<td>100</td>
<td>115-07-1</td>
</tr>
</tbody>
</table>

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

Description of necessary first aid measures

Eye contact: Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.

Inhalation: Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or wristband.

Skin contact: Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.

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

Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact: No known significant effects or critical hazards.

Inhalation: No known significant effects or critical hazards.

Skin contact: No known significant effects or critical hazards.

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

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

Over-exposure signs/symptoms
Section 4. First aid measures

Eye contact : No specific data.
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Indication of immediate medical attention and special treatment needed, if necessary
Notes to physician : Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
Specific treatments : No specific treatment.
Protection of first-aiders : No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

Extinguishing media
Suitable extinguishing media : Use an extinguishing agent suitable for the surrounding fire.
Unsuitable extinguishing media : None known.

Specific hazards arising from the chemical : Contains gas under pressure. Extremely 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.
Hazardous thermal decomposition products : Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Special protective actions for fire-fighters : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Contact supplier immediately for specialist advice. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. If involved in fire, shut off flow immediately if it can be done without risk. If this is impossible, withdraw from area and allow fire to burn. Fight fire from protected location or maximum possible distance. Eliminate all ignition sources if safe to do so.

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, protective equipment and emergency procedures
For non-emergency personnel : Accidental releases pose a serious fire or explosion hazard. No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Shut off all ignition sources. No fires, smoking or flames in hazard area. Avoid breathing gas. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

For emergency responders : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

Date of issue/Date of revision : 7/27/2015.
Section 6. Accidental release measures

Environmental precautions: Ensure emergency procedures to deal with accidental gas releases are in place to avoid contamination of the environment. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods and materials for containment and cleaning up

Small spill: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment.

Large spill: 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

Precautions for safe handling

Protective measures: Put on appropriate personal protective equipment (see Section 8). Contains gas under pressure. Avoid contact with eyes, skin and clothing. Avoid breathing gas. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Empty containers retain product residue and can be hazardous. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Advice on general occupational hygiene: Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

Conditions for safe storage, including any incompatibilities: Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Eliminate all ignition sources. Keep container tightly closed and sealed until ready for use. 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

Control parameters

Occupational exposure limits

<table>
<thead>
<tr>
<th>Ingredient name</th>
<th>Exposure limits</th>
</tr>
</thead>
</table>

Appropriate 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.

Date of Issue/Date of revision: 7/27/2015. Date of previous issue: 10/16/2014. Version: 0.04 4/12
Section 8. Exposure controls/personal protection

Environmental exposure controls: Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures

Hygiene measures: Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection: 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, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with shields.

Skin protection

Hand protection: 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. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection: 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. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.

Other skin protection: Appropriate footwear and any additional skin protection measures 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 protection: 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.

Section 9. Physical and chemical properties

Appearance

Physical state: Gas. [Liquefied compressed gas.]
Color: Colorless.
Molecular weight: 42.09 g/mole
Molecular formula: C3-H6
Boiling/condensation point: -48°C (-54.4°F)
Melting/freezing point: -185°C (-301°F)
Critical temperature: 91.85°C (197.3°F)
Odor: Mild.
Odor threshold: Not available.
PH: Not available.
Flash point: Closed cup: -107.78°C (-162°F)
Burning time: Not applicable.

Date of issue/Date of revision: 7/27/2015.
Date of previous issue: 10/16/2014.
Version: 0.04.
5/12
### Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burning rate</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>Not available.</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.</td>
</tr>
</tbody>
</table>
| Lower and upper explosive (flammable) limits  | Lower: 2%  
Upper: 11%                                                   |
| Vapor pressure                                | 136.6 (psig)                                                        |
| Vapor density                                 | 1.5 (Air = 1)                                                       |
| Specific Volume (ft³/lb)                      | 9.0909                                                              |
| Gas Density (lb/ft³)                          | 0.11 (25°C / 77 to °F)                                             |
| Relative density                              | Not applicable.                                                     |
| Solubility                                    | Not available.                                                      |
| Solubility in water                           | 0.2 g/l                                                             |
| Partition coefficient: n-octanol/water        | 1.77                                                                |
| Auto-ignition temperature                     | 455°C (851°F)                                                       |
| Decomposition temperature                     | Not available.                                                      |
| SADT                                          | Not available.                                                      |
| Viscosity                                     | Not applicable.                                                     |

### Section 10. Stability and reactivity

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactivity</td>
<td>No specific test data related to reactivity available for this product or its ingredients.</td>
</tr>
<tr>
<td>Chemical stability</td>
<td>The product is stable.</td>
</tr>
<tr>
<td>Possibility of hazardous reactions</td>
<td>Under normal conditions of storage and use, hazardous reactions will not occur.</td>
</tr>
<tr>
<td>Conditions to avoid</td>
<td>Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.</td>
</tr>
<tr>
<td>Incompatibility with various substances</td>
<td>Extremely reactive or incompatible with the following materials: oxidizing materials.</td>
</tr>
<tr>
<td>Hazardous decomposition products</td>
<td>Under normal conditions of storage and use, hazardous decomposition products should not be produced.</td>
</tr>
<tr>
<td>Hazardous polymerization</td>
<td>Under normal conditions of storage and use, hazardous polymerization will not occur.</td>
</tr>
</tbody>
</table>

### Section 11. Toxicological information

**Information on toxicological effects**

- **Acute toxicity**
  Not available.

- **Irritation/Corrosion**
  Not available.
Section 11. Toxicological information

Sensitization
Not available.

Mutagenicity
Not available.

Carcinogenicity
Not available.

Classification

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>OSHA</th>
<th>IARC</th>
<th>NTP</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene</td>
<td>-</td>
<td>3</td>
<td>-</td>
</tr>
</tbody>
</table>

Reproductive toxicity
Not available.

Teratogenicity
Not available.

Specific target organ toxicity (single exposure)
Not available.

Specific target organ toxicity (repeated exposure)
Not available.

Aspiration hazard
Not available.

Information on the likely routes of exposure
Not available.

Potential acute health effects

Eye contact : No known significant effects or critical hazards.
Inhalation : No known significant effects or critical hazards.
Skin contact : No known significant effects or critical hazards.
Ingestion : As this product is a gas, refer to the inhalation section.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : No specific data.
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure
Potential immediate effects : Not available.
Potential delayed effects : Not available.

Long term exposure
Potential immediate effects : Not available.
Potential delayed effects : Not available.
Section 11. Toxicological information

Potential chronic health effects
Not available.

- General: No known significant effects or critical hazards.
- Carcinogenicity: No known significant effects or critical hazards.
- Mutagenicity: No known significant effects or critical hazards.
- Teratogenicity: No known significant effects or critical hazards.
- Developmental effects: No known significant effects or critical hazards.
- Fertility effects: No known significant effects or critical hazards.

Numerical measures of toxicity
Acute toxicity estimates
Not available.

Section 12. Ecological information

Toxicity
Not available.

Persistence and degradability
Not available.

Bioaccumulative potential

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>LogP_{ow}</th>
<th>BCF</th>
<th>Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene</td>
<td>1.77</td>
<td>-</td>
<td>low</td>
</tr>
</tbody>
</table>

Mobility in soil

- Soil/water partition coefficient (K_{OC}): Not available.

Other adverse effects
No known significant effects or critical hazards.

Section 13. Disposal considerations

Disposal methods
The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Empty Airegas-owned pressure vessels should be returned to Airegas. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Empty containers or liners may retain some product residues. Do not puncture or incinerate container.
Section 14. Transport information

<table>
<thead>
<tr>
<th>DOT</th>
<th>TDG</th>
<th>Mexico</th>
<th>IMDG</th>
<th>IATA</th>
</tr>
</thead>
<tbody>
<tr>
<td>UN number</td>
<td>UN1077</td>
<td>UN1077</td>
<td>UN1077</td>
<td>UN1077</td>
</tr>
<tr>
<td>UN proper shipping name</td>
<td>PROPYLENE</td>
<td>PROPYLENE</td>
<td>PROPYLENE</td>
<td>PROPYLENE</td>
</tr>
<tr>
<td>Transport hazard class(es)</td>
<td>2.1</td>
<td>2.1</td>
<td>2.1</td>
<td>2.1</td>
</tr>
</tbody>
</table>

Packing group: -
Environment: No.

Additional information:
- Limited quantity: Yes.
- Packaging instruction:
  - Passenger aircraft: Quantity limitation: Forbidden.
  - Cargo aircraft: Quantity limitation: 150 kg
- Special provisions: 19, 190
- Explosive Limit and Limited Quantity Index: 0.128
- ERAP Index: 3000
- Passenger Carrying Ship Index: Forbidden
- Passenger Carrying Road or Rail Index: Forbidden
- Special provisions: 29
- "Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Special precautions for user: Transport within user's premises: always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code: Not available.

Section 15. Regulatory information

- U.S. Federal regulations:
  - TSCA 8(a) CDR Exempt/Partial exemption: Not determined
  - United States inventory (TSCA 8b): This material is listed or exempted.
  - Clean Air Act (CAA) 112 regulated flammable substances: propylene

- Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs): Not listed
- Clean Air Act Section 602 Class I Substances: Not listed
- Clean Air Act Section 602 Class II Substances: Not listed
- DEA List I Chemicals (Precursor Chemicals): Not listed

Date of issue/Date of revision: 7/27/2015
Date of previous issue: 10/16/2014
Version: 0.04
Section 15. Regulatory information

DEA List II Chemicals: Not listed
(Essential Chemicals)

SARA 302/304
Composition/information on ingredients
No products were found.

SARA 304 RQ: Not applicable.

SARA 311/312
Classification: Fire hazard
Sudden release of pressure

Composition/information on ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>%</th>
<th>Fire hazard</th>
<th>Sudden release of pressure</th>
<th>Reactive</th>
<th>Immediate (acute) health hazard</th>
<th>Delayed (chronic) health hazard</th>
</tr>
</thead>
<tbody>
<tr>
<td>propylene</td>
<td>100</td>
<td>Yes.</td>
<td>Yes.</td>
<td>No.</td>
<td>No.</td>
<td>No.</td>
</tr>
</tbody>
</table>

SARA 313

<table>
<thead>
<tr>
<th>Product name</th>
<th>CAS number</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form R - Reporting requirements</td>
<td>propylene</td>
<td>115-07-1</td>
</tr>
<tr>
<td>Supplier notification</td>
<td>propylene</td>
<td>115-07-1</td>
</tr>
</tbody>
</table>

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

State regulations

Massachusetts: This material is listed.
New York: This material is not listed.
New Jersey: This material is listed.
Pennsylvania: This material is listed.
Canada inventory: This material is listed or exempted.

International regulations

International lists:
- Australia inventory (AICS): This material is listed or exempted.
- China inventory (IECSC): This material is listed or exempted.
- Japan inventory: This material is listed or exempted.
- Korea inventory: This material is listed or exempted.
- Malaysia Inventory (EHS Register): Not determined.
- New Zealand Inventory of Chemicals (NZIoC): This material is listed or exempted.
- Philippines inventory (PICCS): This material is listed or exempted.
- Taiwan Inventory (CSNN): Not determined.

Chemical Weapons Convention List Schedule I Chemicals: Not listed
Chemical Weapons Convention List Schedule II Chemicals: Not listed
Chemical Weapons Convention List Schedule III Chemicals: Not listed
Section 15. Regulatory information

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

Canada Label requirements
- Class A: Compressed gas.
- Class B-1: Flammable gas.
- Class D-2B: Material causing other toxic effects (Toxic).

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

<table>
<thead>
<tr>
<th>Health</th>
<th>Flammability</th>
<th>Physical hazards</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks. Although HMIS® ratings are not required on SDSs under 29 CFR 1910. 1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered mark of the National Paint & Coatings Association (NPCA). HMIS® materials may be purchased exclusively from J. J. Keller (800) 327-6868.

The customer is responsible for determining the PPE code for this material.

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

<table>
<thead>
<tr>
<th>Flammability</th>
<th>Instability/Reactivity</th>
<th>Special</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

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Copyright ©2001, National Fire Protection Association, Quincy, MA 02269. This warning system is intended to be interpreted and applied only by properly trained individuals to identify fire, health and reactivity hazards of chemicals. The user is referred to certain limited number of chemicals with recommended classifications in NFPA 49 and NFPA 325, which would be used as a guideline only. Whether the chemicals are classified by NFPA or not, anyone using the 704 systems to classify chemicals does so at their own risk.

History
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Date of issue/Date of revision: 7/27/2015.
Date of previous issue: 10/16/2014.
Version: 0.04
Section 16. Other information

Key to abbreviations:
ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
LogPow = logarithm of the octanol/water partition coefficient
UN = United Nations
ACGIH – American Conference of Governmental Industrial Hygienists
AIHA – American Industrial Hygiene Association
CAS – Chemical Abstract Services
CEPA – Canadian Environmental Protection Act
CERCLA – Comprehensive Environmental Response, Compensation, and Liability Act (EPA)
CPR – Controlled Products Regulations
DSL – Domestic Substances List
GWP – Global Warming Potential
IARC – International Agency for Research on Cancer
ICAO – International Civil Aviation Organisation
Inh – Inhalation
LC – Lethal concentration
LD – Lethal dosage
NDSL – Non-Domestic Substances List
NIOSH – National Institute for Occupational Safety and Health
TDG – Canadian Transportation of Dangerous Goods Act and Regulations
TLV – Threshold Limit Value
TSCA – Toxic Substances Control Act
WEEL – Workplace Environmental Exposure Level
WHMIS – Canadian Workplace Hazardous Material Information System

References:
Not available.

* Indicates information that has changed from previously issued version.

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
Water MSDS

Section 1: Chemical Product and Company Identification

Product Name: Water
Catalog Codes: SLW1063
CAS#: 7732-18-5
RTECS: ZC0110000
TSCA: TSCA 8(b) inventory: Water
Cl#: Not available.
Synonym: Dihydrogen oxide
Chemical Name: Water
Chemical Formula: H2O

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:
1-800-424-3300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>7732-18-5</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

Potential Acute Health Effects:

Potential Chronic Health Effects:

Section 4: First Aid Measures

Eye Contact: Not applicable.
Skin Contact: Not applicable.
Serious Skin Contact: Not available.
Inhalation: Not applicable.
Serious Inhalation: Not available.
Ingestion: Not Applicable
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: Not applicable.
Explosion Hazards in Presence of Various Substances: Not Applicable
Fire Fighting Media and Instructions: Not applicable.
Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures
Small Spill: Mop up, or absorb with an inert dry material and place in an appropriate waste disposal container.
Large Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Section 7: Handling and Storage
Precautions: No specific safety phrase has been found applicable for this product.
Storage: Not applicable.

Section 8: Exposure Controls/Personal Protection
Engineering Controls: Not Applicable
Personal Protection: Safety glasses. Lab coat.
Personal Protection in Case of a Large Spill: Not Applicable
Exposure Limits: Not available.

Section 9: Physical and Chemical Properties
Physical state and appearance: Liquid.
**Odor:** Odorless.
**Taste:** Not available.
**Molecular Weight:** 18.02 g/mole
**Color:** Colorless.
**pH (1% soln/water):** 7 [Neutral.]
**Boiling Point:** 100°C (212°F)
**Melting Point:** Not available.
**Critical Temperature:** Not available.
**Specific Gravity:** 1 (Water = 1)
**Vapor Pressure:** 2.3 kPa (@ 20°C)
**Vapor Density:** 0.62 (Air = 1)
**Volutility:** Not available.
**Odor Threshold:** Not available.
**Water/Oil Dist. Coeff.:** Not available.
**Ionicity (in Water):** Not available.
**Dispersion Properties:** Not applicable
**Solubility:** Not Applicable

### 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:** Not available.
**Special Remarks on Reactivity:** Not available.
**Special Remarks on Corrosivity:** Not available.
**Polymerization:** Will not occur.

### Section 11: Toxicological Information

**Routes of Entry:** Absorbed through skin. Eye contact.

**Toxicity to Animals:**
LD50: [Rat] - Route: oral; Dose: > 90 mL/kg LC50: Not available.

**Chronic Effects on Humans:** Not available.

**Other Toxic Effects on Humans:**

**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 product itself and its products of degradation are not toxic.
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: Not a DOT controlled material (United States).
Identification: Not applicable.
Special Provisions for Transport: Not applicable.

**Section 15: Other Regulatory Information**

Federal and State Regulations: TSCA 8(b) inventory; Water
Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.
Other Classifications:
WHMIS (Canada): Not controlled under WHMIS (Canada).
DSCL (EEC): This product is not classified according to the EU regulations. Not applicable.
HMIS (U.S.A.):
  Health Hazard: 0
  Fire Hazard: 0
  Reactivity: 0
  Personal Protection: a
National Fire Protection Association (U.S.A.):
  Health: 0
  Flammability: 0
  Reactivity: 0
  Specific hazard:
Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM

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

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
## Material Safety Data Sheet
### Acrolein MSDS

### Section 1: Chemical Product and Company Identification

<table>
<thead>
<tr>
<th>Product Name: Acrolein</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalog Codes: SLA1603</td>
</tr>
<tr>
<td>CAS#: 107-02-8</td>
</tr>
<tr>
<td>RTECS: AS1050000</td>
</tr>
<tr>
<td>TSCA: TSCA 8(b) inventory: Acrolein</td>
</tr>
<tr>
<td>CI#: Not applicable.</td>
</tr>
<tr>
<td>Synonym: 2-Propanal; Acraldehyde; Acryaldehyde; Acrylic Aldehyde; Aqualin; Allyl aldehyde; Aqualine; Biocide; Crolean; Ethylene aldehyde; Magnacide; Prop-2-enal</td>
</tr>
<tr>
<td>Chemical Name: Acrolein</td>
</tr>
<tr>
<td>Chemical Formula: H2C=CHCHO or C3-H4-O</td>
</tr>
<tr>
<td>Contact Information: ScienceLab.com, Inc.</td>
</tr>
<tr>
<td>14025 Smith Rd.</td>
</tr>
<tr>
<td>Houston, Texas 77396</td>
</tr>
<tr>
<td>US Sales: 1-800-901-7247</td>
</tr>
<tr>
<td>International Sales: 1-281-441-4400</td>
</tr>
<tr>
<td>Order Online: ScienceLab.com</td>
</tr>
<tr>
<td>CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300</td>
</tr>
<tr>
<td>International CHEMTREC, call: 1-703-527-3887</td>
</tr>
<tr>
<td>For non-emergency assistance, call: 1-281-441-4400</td>
</tr>
</tbody>
</table>

### Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acrolein</td>
<td>107-02-8</td>
<td>100</td>
</tr>
</tbody>
</table>

**Toxicological Data on Ingredients:** Acrolein: ORAL (LD50): Acute: 26 mg/kg [Rat], 13.9 mg/kg [Mouse], 7 mg/kg [Rabbit]. DERMAL (LD50): Acute: 200 mg/kg [Rabbit], VAPOR (LC50): Acute: 18 mg/m4 hours [Rat], 66 ppm 8 hours [Mouse].

### Section 3: Hazards Identification

**Potential Acute Health Effects:**
Very hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Hazardous in case of skin contact (permeator). 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. 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: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY:
Not available. The substance is toxic to lungs, upper respiratory tract. The substance may be toxic to skin, eyes. 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. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. 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:**
If swallowed, 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 immediately.

**Serious Ingestion:** Not available.

Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 220°C (428°F)

**Flash Points:** CLOSED CUP: -26°C (-4.6°F). OPEN CUP: -18°C (-0.4°F) (Cleveland).

**Flammable Limits:** LOWER: 2.8% UPPER: 31%

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

**Fire Hazards in Presence of Various Substances:**
Highly flammable in presence of open flames and sparks, of heat. Flammable in presence of oxidizing materials.

**Explosion Hazards in Presence of Various Substances:**

**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.

**Special Remarks on Fire Hazards:**
Vapors may form explosive mixtures with air. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits toxic fumes of carbon monoxide, peroxides.
Special Remarks on Explosion Hazards: Vapors may form explosive mixtures with air.

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; dixie 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 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, 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). Do not store above 8°C (46.4°F). Refrigerate. Sensitive to light.

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:

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: 0.1 STEL: 0.3 from ACGIH (TLV) [United States] TWA: 0.23 STEL: 0.69 from ACGIH (TLV) [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor:
Disagreeable and choking. Piercing. Extremely sharp. Extremely acrid, pungent, burnt sweet, hot fat

Taste:
Not available.

Molecular Weight: 56.06 g/mole

Color:
Colorless to light yellow.
**pH (1% soln/water):** 7 [Neutral.]
**Boiling Point:** 52.5°C (126.5°F)
**Melting Point:** -88°C (-126.4°F)
**Critical Temperature:** 254°C (489.2°F)
**Specific Gravity:** 0.8389 (Water = 1)
**Vapor Pressure:** 28 kPa (@ 20°C)
**Vapor Density:** 1.94 (Air = 1)
**Volatile:** Not available.
**Odor Threshold:** 0.21 ppm
**Water/Oil Dist. Coeff.:** The product is equally soluble in oil and water; log(oil/water) = 0
**Ionicity (in Water):** Not available.
**Dispersion Properties:** See solubility in water, diethyl ether.
**Solubility:** Soluble in cold water, hot water, diethyl ether. Soluble in petroleum ether, alcohol, oxygenated solvents. Miscible with lower alcohols, ketones, benzene. Solubility in water: 208 g/kg @ 20 deg. C; 212,000 mg/l @ 25 deg. C

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### Section 10: Stability and Reactivity Data

**Stability:** The product is stabilized with Hydroquinone. However, it may form unstable peroxides over time.

**Instability Temperature:** Not available.

**Conditions of Instability:** Heat, ignition sources, incompatible materials, light.

**Incompatibility with various substances:** Reactive with oxidizing agents, acids, alkalis.

**Corrosivity:** Non-corrosive in presence of glass.

**Special Remarks on Reactivity:**
Incompatible with amines. Incompatible with oxygen and peroxides. May polymerize on exposure to light, or in presence of alkali or strong acid forming disacryl. Incompatible with oleum, ethyleneimine, chlorosulfonic acid, ammonium hydroxide, 2-aminoethanol, alkalis, strong acids, mineral acids, oxidizers, ammonia. May form shock sensitive peroxides overtime. Polymerizes readily unless inhibited (stabilized)

**Special Remarks on Corrosivity:** Non-corrosive to iron and steel at room temperature

**Polymerization:**
Will not occur with the product as is. This product is stabilized with Hydroquinone. However, it will polymerize of not stabilized, or in contact with acids (including sulfur dioxide), alkalis, volatile amines, salts, thiourea, oxidants (air), ash on exposure to light and heat.

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### Section 11: Toxicological Information

**Routes of Entry:** Absorbed through skin. Dermal contact. 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): 7 mg/kg [Rabbit]. Acute dermal toxicity (LD50): 200 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 18 mg/ m³ 4 hours [Rat].

**Chronic Effects on Humans:**
CARCINOGENIC EFFECTS: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. Causes damage to the following organs: lungs, upper respiratory tract. May cause damage to the following organs: skin, eyes.
Other Toxic Effects on Humans:
Very hazardous in case of skin contact (irritant), of ingestion. Hazardous in case of skin contact (permeator), of inhalation (lung corrosive). 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. May affect genetic material (mutagenic).

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes severe irritation. May cause skin burns. May be fatal if absorbed through skin. Eyes: Causes severe irritation. May cause corneal burns. It is a lacrimating agent. Inhalation: May be fatal if inhaled. It causes respiratory tract irritation. It is a severe pulmonary irritant. Symptoms may include difficulty breathing (dyspnea), chest congestion, bronchospasm. Delayed of acute lung injury (acute pulmonary edema, emphysema), permanent lung damage may also occur. Nausea, vomiting, and CNS can also occur. Death may result from acute lung injury and/or respiratory failure. Ingestion: May be fatal if swallowed. May produce severe irritation of the mouth, and gastrointestinal tract. It may also affect behavior/central nervous system (general anesthetic, somolence). Other effects may include increase in blood pressure and heart rate. Chronic Potential Health Effects:

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. CLASS 6.1: Poisonous material.

Identification: Acrolein, stabilized UNNA: 1092 PG: I

Special Provisions for Transport:
Marine Pollutant. Inhalation Hazard Zone A

Section 15: Other Regulatory Information

Federal and State Regulations:
Other Regulations:

Other Classifications:
WHMIS (Canada):

DSCL (EEC):
R11- Highly flammable. R24/25- Toxic in contact with skin and if swallowed. R26- Very toxic by inhalation. R34- Causes burns. R50- Very toxic to aquatic organisms. S23- Do not breathe gas/fumes/vapour/spray [**] 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 [**] S39/37/39- Wear suitable protective clothing, gloves and eye/face protection. S45- In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). S61- Avoid release to the environment. Refer to special instructions/Safety data sheets.

HMIS (U.S.A.):
Health Hazard: 3
Fire Hazard: 3
Reactivity: 0
Personal Protection:

National Fire Protection Association (U.S.A.):
Health: 4
Flammability: 3
Reactivity: 3
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:

Other Special Considerations: Not available.

Created: 10/09/2005 03:37 PM
Last Updated: 05/21/2013 12:00 PM

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Material Safety Data Sheet
Acrylic Acid MSDS

Section 1: Chemical Product and Company Identification

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<thead>
<tr>
<th>Product Name:</th>
<th>Acrylic Acid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalog Codes:</td>
<td>SLA3406</td>
</tr>
<tr>
<td>CAS#:</td>
<td>79-10-7</td>
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<tr>
<td>RTECS:</td>
<td>AS4375000</td>
</tr>
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<td>TSCA:</td>
<td>TSCA 8(b) inventory: Acrylic Acid</td>
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<tr>
<td>Cl#:</td>
<td>Not available.</td>
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<tr>
<td>Synonym:</td>
<td>Propenoic Acid Ethylenecarboxylic Acid</td>
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<tr>
<td>Chemical Name:</td>
<td>Acrylic Acid</td>
</tr>
<tr>
<td>Chemical Formula:</td>
<td>C3-H4-O2</td>
</tr>
</tbody>
</table>

Contact Information:

- ScienceLab.com, Inc.
  14025 Smith Rd.
  Houston, Texas 77386
- 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

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
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<tbody>
<tr>
<td>Acrylic Acid</td>
<td>79-10-7</td>
<td>100</td>
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</table>

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, CO2).

**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 spilt 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:**

**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 (286.8°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)
Volutility: 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 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.

Created: 10/09/2005 03:37 PM

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

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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
| Cl#: 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

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
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<tr>
<td>Acetaldehyde</td>
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</table>

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.


Flash Points:
CLOSED CUP: -38°C (-36.4°F) (Buvardi (1996); Clayton and Clayton, 1993; Lewis, 1996); -38.89 deg. C (American Conference of Governmental Industrial Hygienists) 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 Governmental Industrial Hygienists); 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:

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 acid 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.

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### 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).

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### 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:**
Split 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:**
Split 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.

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### 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)
Volutility: 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, ignition 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), acetic anhydrides, alcohols, iodine, isocyanates, phosphorus, phosphorus isocyanate, tris(2-chlorobutyl)amine. It can slowly polymerize to paraaldehyde. 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 affect respiration (dyspnea) and respiratory arrest and death may occur. It may affect behavior/central nervous and cause central nervous system depression. Irritation 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 (b) inventory: Acetaldehyde SARA 313 toxic chemical notification and release reporting: Acetaldehyde CERCLA: Hazardous substances; Acetaldehyde: 1000 lbs. (453.6 kg)

Other Regulations:

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):

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.

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Section 16: Other Information

References:

Other Special Considerations: Not available.

Created: 10/09/2005 03:35 PM
Last Updated: 05/21/2013 12:00 PM

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Material Safety Data Sheet
Propylene oxide MSDS

Section 1: Chemical Product and Company Identification

Product Name: Propylene oxide
Catalog Codes: SLP2539
CAS#: 75-56-9
RTECS: T22975000
TSCA: TSCA 8(b) inventory: Propylene oxide
CI#: Not available.
Synonym:
Chemical Formula: C3H6O

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:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propylene oxide</td>
<td>75-56-9</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Propylene oxide: ORAL (LD50): Acute: 380 mg/kg [Rat]. 440 mg/kg [Mouse]. DERMAL (LD50): Acute: 1500 mg/kg [Rabbit]. VAPOR (LC50): Acute: 4000 ppm 4 hour(s) [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of ingestion, of inhalation. Hazardous in case of skin contact (irritant, permeator). Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
Very hazardous in case of eye contact (irritant), of ingestion, of inhalation. Hazardous in case of skin contact (irritant, permeator). CARCINOGENIC EFFECTS: Classified 2 (Reasonably anticipated.) by NTP. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, mucous membranes. 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. Do not use an eye ointment. Seek medical attention.

**Skin Contact:**
After contact with skin, wash immediately with plenty of water. 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. Cover the irritated skin with an emollient. 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:** Not available.

**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.

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### Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 449°C (840.2°F)

**Flash Points:** CLOSED CUP: -37°C (-34.6°F).

**Flammable Limits:** LOWER: 2.3%  UPPER: 36%

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

**Fire Hazards in Presence of Various Substances:**
Flammable in presence of open flames and sparks. Slightly flammable to 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.

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### 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. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

**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. Eliminate all ignition sources. 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 away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/vapour/spray. 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. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

**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: 20 (ppm) from ACGIH (TLV) TWA: 48 (mg/m3) from ACGIH Consult local authorities for acceptable exposure limits.

**Section 9: Physical and Chemical Properties**

**Physical state and appearance:** Liquid.

**Odor:** Not available.

**Taste:** Not available.

**Molecular Weight:** 58.08 g/mole

**Color:** Not available.

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

**Boiling Point:** 34.23°C (93.6°F)

**Melting Point:** -112°C (-169.6°F)

**Critical Temperature:** Not available.

**Specific Gravity:** 0.83 (Water = 1)

**Vapor Pressure:** 442 mm of Hg (@ 20°C)

**Vapor Density:** 2 (Air = 1)

**Volatile:** Not available.

**Odor Threshold:** 35 ppm

**Water/Oil Dist. Coeff.:** The product is more soluble in oil; log(oil/water) = 0.9

**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: No.

Section 11: Toxicological Information

Routes of Entry: Dermal contact. 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): 380 mg/kg [Rat]. Acute dermal toxicity (LD50): 1500 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 4000 ppm 4 hour(s) [Rat].
Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified 2 (Reasonably anticipated.) by NTP. The substance is toxic to lungs, mucous membranes.
Other Toxic Effects on Humans:
Very hazardous in case of ingestion, of inhalation. Hazardous in case of skin contact (irritant, 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 as toxic as the original product.
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information
**DOT Classification:** Class 3: Flammable liquid.

**Identification:** Propylene oxide: UN1280 PG: I

**Special Provisions for Transport:** Not available.

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### 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: Propylene oxide 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: Propylene oxide Pennsylvania RTK: Propylene oxide Massachusetts RTK: Propylene oxide TSCA 8(b) inventory: Propylene oxide SARA 302/304/311/312 extremely hazardous substances: Propylene oxide SARA 313 toxic chemical notification and release reporting: Propylene oxide


**Other Classifications:**

**WHMIS (Canada):**
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

**DSCL (EEC):**

**HMIS (U.S.A.):**
- Health Hazard: 3
- Fire Hazard: 4
- Reactivity: 0
- Personal Protection: h

**National Fire Protection Association (U.S.A.):**
- Health: 3
- Flammability: 4
- Reactivity: 2
- 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.

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### Section 16: Other Information

**References:** Not available.

**Other Special Considerations:** Not available.

**Created:** 10/10/2005 08:24 PM

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

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MATERIAL SAFETY DATA SHEET

SECTION 1. PRODUCT IDENTIFICATION

PRODUCT NAME: Oxygen, Compressed
CHEMICAL NAME: Oxygen
SYNONYMS: Oxygen gas, Gaseous Oxygen, GOX
MANUFACTURER: Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195 - 1501
PRODUCT INFORMATION: 1-800-752-1597
MSDS NUMBER: 1012
REVISION DATE: January 1995
REVISION: 5
REVIEW DATE: August 1997**

SECTION 2. COMPOSITION / INFORMATION ON INGREDIENTS

Oxygen is sold as pure product > 99%.
CAS NUMBER: 7782-44-7
EXPOSURE LIMITS:
OSHA: Not established
ACGIH: Not established
NIOSH: Not established

SECTION 3. HAZARD IDENTIFICATION

EMERGENCY OVERVIEW
Oxygen is an odorless, colorless, nonflammable gas stored in cylinders at high pressure. It is an oxidizing gas and vigorously accelerates combustion. Keep away from oils or grease. Rescue personnel should be aware of the extreme fire hazards associated with oxygen-enriched (greater than 23%) atmospheres, and that self contained breathing apparatus (SCBA) may be required.

EMERGENCY TELEPHONE NUMBERS
(800) 523-9374 Continental U.S., Canada and Puerto Rico
(610) 481-7711 other locations

POTENTIAL HEALTH EFFECTS INFORMATION:
INHALATION: Breathing 80% or more oxygen at atmospheric pressure for more than a few hours may cause nasal stuffiness, cough, sore throat, chest pain and breathing difficulty. Breathing oxygen at higher pressure increases the likelihood of adverse effects within a shorter time period. Breathing pure oxygen under pressure may cause lung damage and also central nervous system effects resulting in dizziness, poor coordination, tingling sensation, visual and hearing disturbances, muscular twitching, unconsciousness and convulsions. Breathing oxygen under pressure may cause prolongation of adaptation to darkness and reduced peripheral vision.
EYE / SKIN CONTACT: No adverse effect.
EXPOSURE INFORMATION:

ROUTE OF ENTRY: Inhalation

TARGET ORGANS: Eyes, central nervous system

MEDICAL CONDITIONS AGGRAVATED BY OVEREXPOSURE: Patients with chronic obstructive pulmonary disease retain carbon dioxide abnormally. If oxygen is administered to them, raising the oxygen concentration in the blood depresses their breathing and raises their retained carbon dioxide to a dangerous level.

CARCINOGENIC POTENTIAL: Oxygen is not listed as a carcinogen or potential carcinogen by NTP, IARC, or OSHA Subpart Z.

SECTION 4. FIRST AID

INHALATION: Move victim to fresh air or if in elevated pressures reduce oxygen pressures to one atmosphere. Call a physician. The physician should be advised that the victim has been exposed to a high concentration of oxygen. No treatment is required in the absence of symptoms or high pressure exposure.

EYE / SKIN CONTACT: Not applicable

NOTES TO PHYSICIAN: Animal studies suggest that the administration of certain drugs, including phenothiazine drugs and chloroquine, increase the susceptibility to toxicity from oxygen at high pressures. Animal studies also indicate that vitamin "E" deficiency may increase susceptibility to oxygen toxicity.

Airway obstruction during high oxygen tension may cause alveolar collapse following absorption of the oxygen. Similarly, occlusion of the Eustachian tubes may cause retraction of the eardrum and obstruction of the paranasal sinuses may produce "vacuum-type" headache.

All individuals exposed for long periods to oxygen at high pressure and who exhibit overt oxygen toxicity should have ophthalmologic examinations.

SECTION 5. FIRE AND EXPLOSION

FLASH POINT: Not applicable

AUTOIGNITION: Nonflammable

FLAMMABLE LIMITS: Nonflammable

EXTINGUISHING MEDIA: Oxygen is nonflammable but will support combustion. Use extinguishing media appropriate for surrounding fire.

HAZARDOUS COMBUSTION PRODUCTS: None

SPECIAL FIRE FIGHTING INSTRUCTIONS: Evacuate all personnel from the danger area. If possible, shut off flow of oxygen which is supporting the fire. Immediately cool containers with water spray from maximum distance. When cool move cylinders from fire area, if possible without risk. Self contained breathing apparatus may be required for rescue workers.

UNUSUAL FIRE AND EXPLOSION HAZARDS: Oxygen vigorously accelerates combustion. Some materials which are noncombustible in air will burn in the presence of an oxygen enriched atmosphere (greater than 23%). Fire resistant clothing may burn and offer no protection in oxygen rich atmospheres. Oxygen may form explosive compounds when exposed to combustible materials or oil, grease, and other hydrocarbon materials. Pressure in a container can build up due to heat and it may rupture if pressure relief devices should fail to function. Upon exposure to intense heat or flame cylinder will vent rapidly and/or rupture violently. Most cylinders are designed to vent contents when exposed to elevated temperatures. Pressure in a container can build up due to heat and it may rupture if pressure relief devices should fail to function.
SECTION 6. ACCIDENTAL RELEASE MEASURES

Evacuate all personnel from affected area. Shut off source of oxygen if possible. Increase ventilation to release area. Personnel who have been exposed to high concentrations of oxygen should stay in a well-ventilated or open area for 30 minutes before going into a confined space or near an ignition source. If leak is from container or its valve, call the Air Products emergency telephone number. If leak is in user’s system close cylinder valve and vent pressure before attempting repairs.

SECTION 7. STORAGE AND HANDLING

STORAGE: Cylinders should be stored upright in a well-ventilated, secure area, protected from the weather. Storage area temperatures should not exceed 125 °F (52 °C) and area should be free of combustible materials. Storage should be away from heavily traveled areas and emergency exits. Avoid areas where salt or other corrosive materials are present. Cylinders should be separated from flammables by a minimum distance of 20 ft. or by a barricade of non-combustible material at least five ft. high having a fire resistance rating of at least 1/2 hour. Valve protection caps and valve outlet seals should remain on cylinders not connected for use. Separate full from empty cylinders. Avoid excessive inventory and storage time. Use a first-in first-out system. Keep good inventory records.

HANDLING: Do not drag, roll, or slide cylinder. Use a suitable handtruck designed for cylinder movement. Never attempt to lift a cylinder by its cap. Secure cylinders at all times while in use. Use a pressure reducing regulator or separate control valve to safely discharge gas from cylinder. Use a check valve to prevent reverse flow into cylinder. Do not overhear cylinder to increase pressure or discharge rate. Always open cylinder valve slowly. Do not use rapid opening valves (i.e., ball valves). If user experiences any difficulty operating cylinder valve, discontinue use and contact supplier. Never insert an object (e.g., wrench, screwdriver, pry bar, etc.) into valve cap openings. Doing so may damage valve causing a leak to occur. Use an adjustable strap-wrench to remove overtight or rusted caps.

All gauges, valves, regulators, piping and equipment to be used in oxygen service must be cleaned for oxygen service in accordance with Compressed Gas Association pamphlet G-4.1. Carbon steel, stainless steel, copper, brass, nickel and their alloys are materials of construction that can be used in oxygen service. Use piping and equipment adequately designed to withstand pressures to be encountered. Oxygen is not to be used as a substitute for compressed air. Never use an oxygen jet for cleaning purposes of any sort, especially clothing, as it increases the likelihood of an engulfing fire. Use a check valve or other protective apparatus in any line or piping from the cylinder to prevent reverse flow.

When used in welding and cutting read and understand the manufacturer’s instructions and the precautionary label on the products. Never strike an arc on a compressed gas cylinder or make a cylinder a part of an electrical circuit.

SPECIAL REQUIREMENTS: Always store and handle compressed gases in accordance with Compressed Gas Association, Inc. (ph. 703-412-0900) pamphlet CGA P-1, Safe Handling of Compressed Gases in Containers. Local regulations may require specific equipment for storage or use.

CAUTION: Compressed gas cylinders shall not be refilled except by qualified producers of compressed gases. Shipment of a compressed gas cylinder which has not been filled by the owner or with the owner’s written consent is a violation of federal law.

SECTION 8. PERSONAL PROTECTION / EXPOSURE CONTROL

ENGINEERING CONTROLS: Provide ventilation and/or local exhaust to prevent accumulation of high concentrations of gas (greater than 23%).

RESPIRATORY PROTECTION:

GENERAL USE: None required

EMERGENCY: Use SCBA do to possibility of fire when concentrations exceed 23%.
OTHER PROTECTIVE EQUIPMENT: Safety shoes and work gloves are recommended when handling cylinders. Clothing exposed to high concentrations may retain oxygen 30 minutes or longer and become a potential fire hazard. Stay away from ignition sources.
SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE: Colorless gas
ODOR: Odorless
MOLECULAR WEIGHT: 32.0
BOILING POINT (1 atm): -297.3 °F (-183.0 °C)
SPECIFIC GRAVITY (Air =1): 1.10
SPECIFIC VOLUME (at 70 °F 21.1 °C and 1 atm): 12.08 ft³/lb (0.754 m³/kg)
FREEZING / MELTING POINT: -361.9 °F (-218.8 °C)
VAPOR PRESSURE: Not applicable at 70°F
GAS DENSITY (At 70°F (21.1°C) and 1 Atm): 0.083 lb /ft³ (1.326 kg/m³)
SOLUBILITY IN WATER (Vol./Vol. at 32°F (0°C)): 0.049

SECTION 10. REACTIVITY / STABILITY

CHEMICAL STABILITY: Stable
CONDITIONS TO AVOID: None
INCOMPATIBILITY: Oils, grease, hydrocarbons and flammable materials.
HAZARDOUS DECOMPOSITION PRODUCTS: None
HAZARDOUS POLYMERIZATION: Will not occur

SECTION 11. TOXICOLOGICAL INFORMATION

At atmospheric concentration and pressure, oxygen poses no toxicity hazards.
Premature infants exposed to high oxygen concentrations may suffer delayed retinal damage
which can progress to retinal detachment and blindness. Retinal damage may also occur in adults
exposed to 100% oxygen for extended periods (24 to 48 hr).
At two or more atmospheres central nervous system (CNS) toxicity occurs. Symptoms include
nausea, vomiting, dizziness or vertigo, muscle twitching, vision changes, and loss of consciousness
and generalized seizures. At three atmospheres, CNS toxicity occurs in less than two hours, and at
six atmospheres in only a few minutes.

SECTION 12. ECOLOGICAL INFORMATION

The atmosphere contains 21% oxygen. No adverse ecological effects are expected. Oxygen does not
contain any Class I or Class II ozone depleting chemicals. Oxygen is not listed as a marine pollutant by
DOT (49 CFR 171).

SECTION 13. DISPOSAL

UNUSED PRODUCT / EMPTY CONTAINER: Return container and unused product to supplier. Do
not attempt to dispose of residual or unused quantities.
DISPOSAL: For emergency disposal, secure cylinder and slowly discharge gas to the atmosphere
in a well ventilated area or outdoors.

SECTION 14. TRANSPORTATION

DOT HAZARD CLASS: 2.2 (Nonflammable Gas)       DOT SHIPPING LABEL: Nonflammable Gas, Oxidizer
DOT SHIPPING NAME: Oxygen, compressed
IDENTIFICATION NUMBER: UN 1072
REPORTABLE QUANTITY (RQ): None
PLACARD: Nonflammable Gas or Oxygen
**SPECIAL SHIPPING INFORMATION:** Cylinders should be transported in a secure upright position in a well ventilated truck. Never transport in passenger compartment of a vehicle. An oxygen label may be used for domestic shipment in the United States and Canada in place of the Non-flammable and Oxidizer labels (49CFR Part 172).

**SECTION 15. REGULATORY INFORMATION**

**U.S. FEDERAL REGULATIONS:**

**EPA - ENVIRONMENTAL PROTECTION AGENCY:**

**CERCLA:** Comprehensive Environmental Response, Compensation, and Liability Act of 1980 requires notification to the National Response Center of releases of quantities of hazardous substances equal to or greater than the reportable quantities (RQ) in 40 CFR 302.4.

**CERCLA Reportable Quantity:** None

**SARA TITLE III:** Superfund Amendments and Reauthorization Act of 1986

**SECTION 302:** Requires emergency planning based on threshold planning quantities (TPQ) and release reporting based on reportable quantities (RQ) of EPA's extremely hazardous substances (40 CFR 355).

Oxygen is not listed as an Extremely Hazardous Substance.

**SECTIONS 311/312:** Require submission of material safety data sheets (MSDSs) and chemical inventory reporting with identification of EPA defined hazard classes. The hazard classes for this product are:

<table>
<thead>
<tr>
<th>IMMEDIATE</th>
<th>PRESSURE</th>
<th>REACTIVITY</th>
<th>FIRE</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>

**SECTION 313:** Requires submission of annual reports of releases of toxic chemicals that appear in 40 CFR 372.

Oxygen is not listed as a toxic chemical.

**40 CFR PART 68:** Risk Management for Chemical Accident Release Prevention. Requires the development and implementation of risk management programs at facilities that manufacture, use, store, or otherwise handle regulated substances in quantities that exceed specified thresholds.

Oxygen is not listed as a regulated substance.

**TOXIC SUBSTANCE CONTROL ACT (TSCA):** Oxygen is listed on the TSCA inventory.

**OSHA - OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION**

**29 CFR 1910.119:** Process Safety Management of Highly Hazardous Chemicals. Requires facilities to develop a process safety management program based on Threshold Quantities (TQ) of highly hazardous chemicals.

Oxygen is not listed as a Highly Hazardous Chemical.

**STATE REGULATIONS**

**CALIFORNIA:**

Proposition 65: This product does NOT contain any listed substances for which the State of California requires warning under this statute.

**SCAQMD Rule:** VOC = Not applicable
### SECTION 16. SUPPLEMENTAL INFORMATION

<table>
<thead>
<tr>
<th>HAZARD RATINGS:</th>
<th>HMIS RATINGS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>NFPA RATINGS:</td>
<td></td>
</tr>
<tr>
<td>HEALTH: 0</td>
<td>HEALTH: 0</td>
</tr>
<tr>
<td>FLAMMABILITY: 0</td>
<td>FLAMMABILITY: 0</td>
</tr>
<tr>
<td>REACTIVITY: 0</td>
<td>REACTIVITY: 0</td>
</tr>
<tr>
<td>SPECIAL: OX (oxidizer)</td>
<td></td>
</tr>
</tbody>
</table>

**Documents with Revision Date January 1995 and Review Date August 1997 are identical in content and either may be used.**
MATERIAL SAFETY DATA SHEET

SECTION 1. PRODUCT IDENTIFICATION

PRODUCT NAME: Carbon Dioxide
CHEMICAL NAME: Carbon Dioxide
SYNONYMS: Carbonic Anhydride, Carbonic Acid Gas, Carbon Anhydride
MANUFACTURER: Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195-1501

PRODUCT INFORMATION:
MSDS NUMBER: 1005
REVISION DATE: March 1993
REVIEW DATE: March 1994
MSDS NUMBER: 1005
REVISION: 5

SECTION 2. COMPOSITION / INFORMATION ON INGREDIENTS

CONCENTRATION: Carbon dioxide is sold as pure product > 99%.
CAS NUMBER: 124-38-9
EXPOSURE LIMITS:
OSHA: PEL-TWA = 5000 ppm
ACGIH: TLV-TWA = 5000 ppm
NIOSH: None

SECTION 3. HAZARDS IDENTIFICATION

EMERGENCY OVERVIEW
Carbon dioxide is a nonflammable liquefied compressed gas packaged in cylinders under its own vapor pressure of 838 psig at 70 °F (21.1 °C). High concentrations can cause rapid suffocation and can also increase respiration and heart rate. Contact with liquid may cause frostbite. Avoid breathing gas. Self contained breathing apparatus (SCBA) may be required by rescue workers.

EMERGENCY TELEPHONE NUMBERS
800 - 523 - 9374 Continental U.S., Canada, or Puerto Rico
610 - 481 - 7711 other locations

POTENTIAL HEALTH EFFECTS:
INHALATION: Carbon dioxide is an asphyxiant. Concentrations of 10% or more can produce unconsciousness or death.
EYE CONTACT: Contact with liquid or cold vapor can cause freezing of tissue.
SKIN CONTACT: Contact with liquid or cold vapor can cause frostbite.

EXPOSURE INFORMATION:
ROUTE OF ENTRY: Inhalation
TARGET ORGANS: Central nervous system
EFFECT: Asphyxiation (suffocation). Overexposure may cause damage to retinal ganglion cells and central nervous system.
SYMPTOMS: Headache, sweating, rapid breathing, increased heartbeat, shortness of breath, dizziness, mental depression, visual disturbances, and shaking.

CHRONIC EFFECTS: None established.

MEDICAL CONDITIONS AGGRAVATED BY OVEREXPOSURE: None

CARCINOGENICITY: Carbon dioxide is not listed by NTP, OSHA or IARC.

SECTION 4. FIRST AID

INHALATION: Persons suffering from overexposure should be moved to fresh air. If victim is not breathing, administer artificial respiration. If breathing is difficult, administer oxygen. Obtain prompt medical attention.

EYE CONTACT: Contact with liquid or cold vapor can cause freezing of tissue. Gently flush eyes with lukewarm water. Obtain medical attention immediately.

SKIN CONTACT: Contact with liquid or cold vapor can cause frostbite. Immediately warm affected area with lukewarm water not to exceed 107 °F.

NOTES TO PHYSICIAN: There is no specific antidote. Treatment for overexposure should be directed at the control of symptoms and the clinical condition.

SECTION 5. FIRE AND EXPLOSION

FLASH POINT: Not Applicable
AUTOIGNITION: Nonflammable
FLAMMABLE LIMITS: Nonflammable

EXTINGUISHING MEDIA: Carbon dioxide is nonflammable and does not support combustion. Carbon dioxide is an extinguishing agent for class B and C fires. Use extinguishing media appropriate for the surrounding fire.

HAZARDOUS COMBUSTION PRODUCTS: None known.

FIRE FIGHTING PROCEDURES: Evacuate personnel from danger area. Carbon dioxide is nonflammable. If possible, without risk, remove cylinders from fire area or cool with water. Self contained breathing apparatus (SCBA) may be required for rescue workers.

UNUSUAL HAZARDS: Upon exposure to intense heat or flame, cylinder will vent rapidly and or rupture violently. Most cylinders are designed to vent contents when exposed to elevated temperatures. Pressure in a container can build up due to heat and it may rupture if pressure relief devices should fail to function.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Evacuate all personnel from affected area. Increase ventilation to release area and monitor oxygen level. Use appropriate protective equipment (SCBA). If leak is from cylinder or cylinder valve call the Air Products emergency telephone number. If leak is in user's system close cylinder valve and vent pressure before attempting repairs.

SECTION 7. HANDLING AND STORAGE

STORAGE: Cylinders should be stored upright in a well-ventilated, secure area, protected from the weather. Storage area temperatures should not exceed 125 °F (52 °C). Storage should be away from heavily traveled areas and emergency exits. Avoid areas where salt or other corrosive materials are present. Valve protection caps and valve outlet seals should remain on cylinders not connected for use. Separate full from empty cylinders. Avoid excessive inventory and storage time. Use a first-in first-out system. Keep good inventory records.

HANDLING: Use a suitable hand truck for cylinder movement. Never attempt to lift a cylinder by its valve protection valve cap. Never apply flame or localized heat directly to any part of the cylinder. Do not
allow any part of the cylinder to exceed 125 °F (52 °C). High temperature may cause damage to cylinder and/or premature failure of pressure relief device which will result in venting of cylinder contents. If user experiences any difficulty operating cylinder valve discontinue use and contact supplier. Never insert an object (e.g., wrench, screwdriver, pry bar, etc.) into valve cap openings. Doing so may damage valve causing a leak to occur. Use an adjustable strap wrench to remove overtight or rusted caps.

Only the proper CGA connections should be used, never use adapters. Use piping and equipment adequately designed to withstand pressures to be encountered. If liquid product is being used ensure steps have been taken to prevent entrapment of liquid in closed systems. The use of pressure relief devices may be necessary. Use a check valve or other protective apparatus in any line or piping from the cylinder to prevent reverse flow.

Carbon dioxide is compatible with all common materials of construction. Pressure requirements should be considered when selecting materials and designing systems.

Use a “FULL”, “IN USE”, and “EMPTY” tag system on cylinders. This will reduce the chances of inadvertently connecting or operating the wrong cylinder.

SPECIAL REQUIREMENTS: Always store and handle compressed gases in accordance with Compressed Gas Association, Inc. (ph. 703-979-0900) pamphlet CGA P-1, Safe Handling of Compressed Gases in Containers. Local regulations may require specific equipment for storage or use.

CAUTION: Compressed gas cylinders shall not be refilled except by qualified producers of compressed gases. Shipment of a compressed gas cylinder which has not been filled by the owner or with the owner’s written consent is a violation of federal law.

SECTION 8. PERSONAL PROTECTION / EXPOSURE CONTROL

ENGINEERING CONTROLS: Provide ventilation and/or local exhaust to prevent accumulation of carbon dioxide concentrations above 5000 ppm.

RESPIRATORY PROTECTION:

Emergency Use: Self contained breathing apparatus (SCBA) or positive pressure airline with mask and escape pack are to be used in oxygen deficient atmosphere. Air purifying respirators will not provide protection.

EYE PROTECTION: Safety glasses are recommended when handling, connecting, or disconnecting cylinders, and when pressurizing systems

OTHER PROTECTIVE EQUIPMENT: Safety shoes and leather work gloves when handling cylinders.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE, ODOR AND STATE: Colorless and odorless. A slightly acid gas. It is felt by some to have a slight pungent odor and biting taste.

MOLECULAR WEIGHT: 44.01

GAS DENSITY (at 70 °F (21.1 °C) and 1 atm): 0.1144 lb/ft³ (1.832 kg/m³)

VAPOR PRESSURE (at 70 °F (21.1 °C)): 838 psig

SPECIFIC GRAVITY (Air =1): 1.522

SPECIFIC VOLUME (at 70 °F (21.1 °C) and 1 atm): 8.74 ft³/lb (0.5457 m³/kg)

BOILING POINT: -109.3 °F (-78.5 °C)

TRIPLE POINT (At 60.4 psig): -69.9 °F (-56.6 °C)

SOLUBILITY IN WATER (Vol./Vol. at 88 °F (20 °C)): 0.90
SECTION 10. STABILITY AND REACTIVITY

STABILITY: Stable
CONDITIONS TO AVOID: None
INCOMPATIBILITY (Materials to Avoid): None
REACTIVITY:
HAZARDOUS DECOMPOSITION PRODUCTS: None
HAZARDOUS POLYMERIZATION: Will not occur

SECTION 11. TOXICOLOGICAL INFORMATION

Carbon dioxide is an asphyxiant. It initially stimulates respiration and then causes respiratory depression. High concentrations result in narcosis. Symptoms in humans are as follows:

<table>
<thead>
<tr>
<th>CONCENTRATION</th>
<th>EFFECT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1%</td>
<td>Slight increase in breathing rate</td>
</tr>
<tr>
<td>2%</td>
<td>Breathing rate increases to 50% above normal. Prolonged exposure can cause headache and tiredness.</td>
</tr>
<tr>
<td>3%</td>
<td>Breathing increases to twice the normal rate and becomes labored. Weak narcotic effect. Impaired hearing, headache, increase in blood pressure and pulse rate.</td>
</tr>
<tr>
<td>4-5%</td>
<td>Breathing increases to approximately four times the normal rate, symptoms of intoxication become evident and slight choking may be felt.</td>
</tr>
<tr>
<td>5-10%</td>
<td>Characteristic sharp odor noticeable. Very labored breathing, headache, visual impairment and ringing in the ears. Judgment may be impaired, followed within minutes by loss of consciousness.</td>
</tr>
<tr>
<td>50-100%</td>
<td>Unconsciousness occurs more rapidly above 10% level. Prolonged exposure to high concentrations may eventually result in death from asphyxiation.</td>
</tr>
</tbody>
</table>

SECTION 12. ECOLOGICAL INFORMATION

No adverse ecological effects are expected. No adverse ecological effects are expected. Carbon dioxide does not contain any Class I or Class II ozone depleting chemicals. Carbon dioxide is not listed as a marine pollutant by DOT (49 CFR 171).

SECTION 13. DISPOSAL

UNUSED PRODUCT / EMPTY CYLINDER: Return cylinder and unused product to supplier. Do not attempt to dispose of unused product. Ensure cylinder valve is properly closed, valve outlet cap has been reinstalled, and valve protection cap is secured before shipping cylinder.

WASTE DISPOSAL METHODS: For emergency disposal, secure the cylinder and slowly discharge gas to the atmosphere in a well ventilated area or outdoors. Small amounts may be disposed of by reacting with a mild base.

SECTION 14. TRANSPORT INFORMATION

DOT SHIPPING NAME: Carbon dioxide
HAZARD CLASS: 2.2 (Nonflammable Gas)
IDENTIFICATION NUMBER: UN1013
PRODUCT RQ: None
SHIPPING LABEL(s): Nonflammable gas
PLACARD (when required): Nonflammable gas
SPECIAL SHIPPING INFORMATION: Cylinders should be transported in a secure upright position in a well ventilated truck. Never transport in passenger compartment of a vehicle.

SECTION 15. REGULATORY INFORMATION

U.S. FEDERAL REGULATIONS:

ENVIRONMENTAL PROTECTION AGENCY (EPA):

CERCLA: Comprehensive Environmental Response, Compensation, and Liability Act of 1980 requires notification to the National Response Center of a release of quantities of hazardous substances equal to or greater than the reportable quantities (RQ’s) in 40 CFR 302.4.

CERCLA Reportable Quantity: None.

SARA TITLE III: Superfund Amendment and Reauthorization Act of 1986

SECTION 302/304: Requires emergency planning on threshold planning quantities (TPQ) and release reporting based on reportable quantities (RQ) of EPA’s extremely hazardous substances (40 CFR 355).

Extremely Hazardous Substances: None
Threshold Planning Quantity (TPQ): None

SECTIONS 311/312: Require submission of material safety data sheets (MSDSs) and chemical inventory reporting with identification of EPA defined hazard classes. The hazard classes for this product are:

IMMEDIATE HEALTH: Yes
PRESSURE: Yes
DELAYED HEALTH: No
REACTIVITY: No
FLAMMABLE: No

SECTION 313: Requires submission of annual reports of release of toxic chemicals that appear in 40 CFR 372.

Carbon dioxide does not require reporting under Section 313

40 CFR Part 68 - Risk Management for Chemical Accident Release Prevention: Requires the development and implementation of risk management programs at facilities that manufacture, use, store, or otherwise handle regulated substances in quantities that exceed specified thresholds.

Carbon dioxide is not listed as a regulated substance.

TSCA - TOXIC SUBSTANCES CONTROL ACT: Carbon dioxide is listed on the TSCA inventory.

OSHA - OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION:


Carbon dioxide is not listed in Appendix A as a highly hazardous chemical.

STATE REGULATIONS:

CALIFORNIA:

Proposition 65: This product does NOT contain any listed substances which the State of California requires warning under this statute.

SCAQMD Rule: VOC = Not applicable
### SECTION 16. OTHER INFORMATION

<table>
<thead>
<tr>
<th>NFPA RATINGS:</th>
<th>HMIS RATINGS:</th>
</tr>
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<tbody>
<tr>
<td>HEALTH: 1</td>
<td>HEALTH: 0</td>
</tr>
<tr>
<td>FLAMMABILITY: 0</td>
<td>FLAMMABILITY: 0</td>
</tr>
<tr>
<td>REACTIVITY: 0</td>
<td>REACTIVITY: 0</td>
</tr>
<tr>
<td>SPECIAL: SA*</td>
<td></td>
</tr>
</tbody>
</table>

*Compressed Gas Association recommendation to designate simple asphyxiant.

APPENDIX D: Patent

United States Patent Application Publication

Bal et al.

PROCESS FOR PREPARATION OF Ag-W OXIDE CATALYST FOR THE SELECTIVE CONVERSION OF PROPIPOLYLENE OXIDE TO PROPYLENE OXIDE WITH MOLECULAR OXYGEN

Applicant: Council of Scientific and Industrial Research, New Delhi (IN)

Inventors: Rajaram Bal, Mohankumar (IN); Shilpi Ghosh, Mohankumar (IN); Gobhira Acharyya Shanka, Mohankumar (IN); Bipul Sackar, Mohankumar (IN); Chandrashekhar Pundem, Mohankumar (IN); Rajib Kumar Singha, Mohankumar (IN)

Appl. No.: 14/566,244
PCT Filed: Dec. 21, 2012
PCT No.: PCT/IN2012/000836
§ 371(c)(1), (2), (4) Date: Jun. 17, 2014

Foreign Application Priority Data

Dec. 27, 2011 (IN) 3824/DEL/2011

Publication Classification

Int. Cl.
B01J 23/48
C07D 307/10

US Cl.
CPC B01J 23/687 (2013.01); C07D 307/10 (2013.01)
USPC 549/534: 423/594.13: 502/317

ABSTRACT

The present invention provides a process for preparation of Ag-W oxide catalyst for the direct and selective conversion of propylene to propylene oxide. The process provides a direct single step selective vapour phase oxidation of propylene to propylene oxide using molecular oxygen over Ag-W oxide catalysts. The process provides propylene conversion of 10-50% and selectivity for propylene oxide up to 100%.
Powder X-Ray Diffraction (XRD)

Fig. 1

Scanning Electron Microscopy (SEM)

Fig. 2
Transmission Electron Microscopy (TEM)

Fig. 5
PROCESS FOR PREPARATION OF Ag-W OXIDE CATALYST FOR THE SELECTIVE CONVERSION OF PROPYLENE TO PROPYLENE OXIDE WITH MOLECULAR OXYGEN

FIELD OF THE INVENTION

[0001] The present invention relates to a process for preparation of Ag₆O₃-WO₃ catalyst for the selective conversion of propylene to propylene oxide with molecular oxygen.

[0002] More particularly, the present invention relates to a process for the selective oxidation of propylene to propylene oxide with molecular oxygen over Ag-W oxide catalyst. More particularly, the present invention relates to a process for the vapour phase selective oxidation of propylene to propylene oxide by using molecular oxygen over Ag-W oxide catalyst.

BACKGROUND OF THE INVENTION

[0003] Propylene oxide (PO) is a versatile chemical intermediate used in a wide range of industrial and commercial products including polyether polyols, propylene glycols and propylene glycol ethers. By volume, it is among the top 50 chemicals produced in the world with the annual production of about 5 million tons. Industrial production of propylene oxide is mainly from co-oxidation of propylene with other chemicals but these technologies create additional side products. The major conventional manufacturing methods of PO are the chlorohydration process and the Halcra process. The chlorohydration process is being phased out because of environmental pollution, while the latter has the by product limitation. So a new technology with environmentally benign has to be developed for the production of propylene oxide. The main concern in the fine chemical and drug intermediates are the amount of waste generated per unit weight of desired product (called E-factor by R A Sheldon in Chemistry & Industry, 6 Jan. 1997, P 13) and poor atom efficiencies (kg of product produced per kg of reactants used) due to the use of stoichiometric reagents and minerals acid/base catalysts. In this context, the use of solid catalysts which are eco-safe and reusable become important. Moreover a major problem with this process is that it produces phenol is driving its price down and also hurting the economics of phenol as well. This concern is the impetus for researchers to develop a direct single step co-product free and environment friendly route to propylene oxide.

[0004] There are reports on the production of propylene oxide by direct oxidation of propylene with different oxidants over different solid catalyst but to the best of our knowledge there is no reference for the use of molecular oxygen only for this purpose.

[0005] Reference may be made to article in the Science 2001, 292, 1139-1141 by Chinese group Zuwei et al the use of H₂O₂ as the oxidizing agent for the conversion of propylene oxide from propylene to achieve ~85% yield over W containing heteropolyacid.

[0006] Reference may be made to article in the Journal of Catalysis 2002, 211, 552-555 by Fan Li and his group reported the use of mixture of H₂ and O₂ for the conversion of propylene to propylene oxide to achieve ~1% conversion and 43% propylene oxide selectivity over NaCl-modified V₃O₅, Cu₃O₅ oxide catalyst.

[0007] Reference may be made to article in the Journal of Phys. Chem. B, 2005, 109, 19309-19319 by Nijhuis et al reported the use of H₂O₂ as oxidants for the conversion of propylene to propylene oxide with ~4% propylene conversion and 93% propylene oxide selectivity over Au supported titania catalyst.

[0008] Reference may be made to article in the Journal of Catalysis, 2005, 232, 85-95, in which Oyama et al and his group reported the use of molecular oxygen for the oxidation of propylene to propylene oxide to achieve ~30 propylene conversion with ~10% propylene oxide selectivity over Ag supported CaCO₃ catalyst.

[0009] Reference may be made to article in the Angew. Chem. Int. Ed. 2004, 43, 1546-1548, in which Japanese worker Prof Haruta and his group reported the use of mixture of H₂O₂ for the oxidation of propylene to propylene oxide to achieve 10% conversion and ~90% selectivity over Ba(NO₃)₂-Auvitanol silicate catalyst.

[0010] Reference may also be made to article in the Angew. Chem. Int. Ed. 2006, 45, 412-415, in which the same Japanese worker Prof Haruta and his group reported the use of mixture of H₂O₂ for the oxidation of propylene to propylene oxide to achieve 9% conversion and ~90% selectivity over gold supported titanate silicate catalyst, where small amount of triethylamine was introduced with the feed mixture.

[0011] Reference may be made to article in the Catalysis Lett. 2007, 119, 185-190 in which Li et al reported the use of molecular oxygen as the oxidizing agent for the oxidation of propylene to propylene oxide to achieve 4% propylene conversion and 46.8% propylene oxide selectivity over Ag-Y₂O₃-K₂O/Al₂O₃ catalyst.

[0012] Reference may also be made to article in the Journal of Phys. Chem. C, 2008, 112, 7731-7734 in which Wang et al reported the use of molecular oxygen as the oxidizing agent to convert propylene to propylene oxide with a propylene conversion of ~4% with a propylene oxide selectivity of 55% over CuO/Al₂O₃ catalyst.

[0013] Reference may also be made to article in the Ind. Eng. Chem. Res. 2010, 49, 2624-2637 in which Bettini et al reported the use of nitrous oxide as the oxidizing agent for the oxidation of propylene to propylene oxide to achieve ~10% conversion and ~75% propylene oxide selectivity over Fe/Si/Al catalyst.

[0014] Reference may also be made to article in the Angew. Chem. Int. Ed. 2009, 48, 1546-1548, in which the same Japanese worker Prof Haruta and his group reported the use of mixture of H₂O₂/O₂ for the oxidation of propylene to propylene oxide to achieve 0.8% conversion and ~5% selectivity over gold supported TS-1 catalyst.

[0015] The drawback of the processes reported so far is that they do not exhibit sufficiently high conversions of propylene for high selectivity of propylene oxide to be of interest for industrial application. In most of the cases hazardous oxidizing agent N₂O, H₂O₂ or expensive H₂ with O₂ was used and also lots of unnecessary by-products was formed. In addition, the catalysts used have a limited activity under the operating conditions. There is, therefore, an evident necessity for further improvements in the process for the selective conversion of propylene to propylene oxide.
OBJECTS OF THE INVENTION

[0016] The main object of the present invention is to provide a process for preparation of Ag—W oxide catalyst for the selective conversion of propylene to propylene oxide with molecular oxygen.

[0017] Another objective of the present invention is to provide a process for the vapor phase selective oxidation of propylene to propylene oxide using oxygen as the oxidant and Ag—W oxide as the catalyst.

[0018] Still another objective of the present invention is to provide a process to obtain propylene oxide from propylene with high selectivity.

[0019] Yet another objective of the present invention is to provide a process which uses environmentally friendly green oxidizing agent, oxygen for the synthesis of propylene oxide.

[0020] Still another objective of the present invention is to provide a process which works under continuous process for the synthesis of propylene oxide.

[0021] Yet another objective of the present invention is to provide a catalyst with the mixture of Ag and W oxide which can be prepared easily and also very economical to produce propylene oxide from propylene.

SUMMARY OF THE INVENTION

[0022] Accordingly, the present invention provides a process for the preparation of Ag—W oxide catalyst, wherein the said process comprising the steps of:

[0023] a. mixing a salt of Ag preferably, AgNO₃, WO₃, 2H₂O, a surfactant preferably, cetyltrimethylammonium bromide (CTAB), a reducing agent, preferably, hydrazine, H₂O to obtain a gel;

[0024] b. mixing gel as obtained in step (a) with constant stirring for 2-6 h at room temperature ranging between 25-35°C;

[0025] c. filtering the gel as obtained in step (b) and washing with excess water and dried in an oven with temperature range of 100-120°C for a period ranging between 6-18 h;

[0026] d. calcining the dried product as obtained in step (c) at temperature range of 300-750°C, for a period ranging between 4-10 h to obtain Ag—W oxide catalyst.

[0027] In an embodiment of the invention, weight ratio of Ag to W in step (a) is in the range of 0.03 to 0.5.

[0028] In one embodiment of the invention, molar ratio of Ag to CTAB in step (a) is in the range of 0.75-1.3.

[0029] In another embodiment of the invention, molar ratio of Ag to hydrazine in step (a) is in the range of 0.75-1.3.

[0030] In yet another embodiment, a process for selective oxidation (epoxidation) of propylene to propylene oxide using Ag—W oxide catalyst wherein the said process comprising the steps of reacting propylene with oxygen in the presence of Ag—W oxide catalyst in the pressure range of 1-5 bar, at a temperature ranging between 150-450°C, with a weight hourly space velocity (WHSV, feed/g catalyst/hour) in the range of 2000 to 30000 h⁻¹ for a period in the range of 1-20 hours to obtain propylene oxide.

[0031] In still another embodiment, the conversion of propylene oxide in the range of 10-50%.

[0032] In still another embodiment, selectivity of the propylene oxide obtained in the range of 80-100%.

[0033] In still another embodiment, the yield of propylene oxide in the range of 10-50%.

[0034] In still another embodiment, Ag—W oxide catalyst having molecular formula AgₓW₁₋ₓOₙ₋₁ which comprises of 2-20 wt % Ag and 60-85% wt % W in wt % and oxygen 5-30 wt %

BRIEF DESCRIPTION OF DRAWING

[0035] FIG. 1 shows the main peaks at 23.22, 24.5, 23.72 and 34.25° (2θ) are due to the WO₃ support (example 1).

[0036] There were four diffraction peaks of Ag at 2θ=38.1, 44.3, 64.4 and 77.4° corresponding to the crystal faces of Ag(111), (200), (220) and (311), respectively, which coincide well with the literature values (JCPDS No. 04-0783).

[0037] FIG. 2 Low magnification SEM image shows that uniform rod-like structure with diameter around 30-40 nm and length up to several microns (example 1).

[0038] FIG. 3 High magnification SEM image shows that Ag nanoparticles supported on uniform rod-like structure with diameter around 30-40 nm and length up to several microns attending a high aspect ratio (example 1).

[0039] FIG. 4 Energy Dispersive X-ray analysis (EDAX) analysis showing the presence of Ag, W, O in the catalyst (example 1).

[0040] FIG. 5 High resolution transmission electron microscopy (HRTEM) revealed a rod-like morphology of tungsten oxide with an average width of 30 nm covered by ordered silver particles with size nearly 5 nm (example 1).

[0041] FIG. 6 Size distribution of silver nanoparticles (example 1).

[0042] FIG. 7 shows the XRD of catalyst prepared in example 2.

[0043] FIG. 8 shows the SEM of catalyst prepared in example 2.

[0044] FIG. 9 shows the TEM of catalyst prepared in example 2.

DETAILED DESCRIPTION OF THE INVENTION

[0045] The present invention provides a process for the preparation of Ag—W oxide (Ag nanoparticles supported on WO₃ nanorods) catalyst by room temperature synthesis for the preparation of propylene oxide by vapor phase selective epoxidation of propylene using oxygen as the oxidant involves the following steps.

[0046] The process for the preparation of Ag—W oxide catalyst comprising the steps of preparation of the gel composition using AgNO₃, WO₃, 2H₂O, cetyltrimethylammonium bromide, hydrazine, H₂O where AgNO₃, WO₃, 2H₂O are the precursors for Ag and W respectively.

[0047] The weight ratio of Ag to W was varied in the range between 0.03 to 0.5.

[0048] The molar ratio of Ag to CTAB varied in the range of 0.75-1.3.

[0049] The molar ratio of Ag to hydrazine varied in the range of 0.75-1.3.

[0050] The mixing gel was stirred for 2-6 h at room temperature.

[0051] The product was filtered with excess water and dried in an oven with temperature range of 100-120°C. The dried product was calcined in a furnace in the temperature range of 300-750°C.
General procedure for the Conversion of Propylene to Propylene Oxide

[0052] The reaction was carried out in a fixed bed down flow high pressure reactor by charging a catalyst for 1 to 30 h to get propylene oxide. The pressure of the reactor was maintained by using oxygen and the oxygen pressure is preferably in the range 2 to 5 MPa. The reaction temperature is preferably in the range 150-400°C. The weight hourly space velocity (WHSV) is preferably in the range 5000 to 20000 edL/hr/gm. Propylene was introduced in the reactor by using mass flow controller. The reaction mixtures were analysed by two online GC’s with an FID detector by using capillary column for hydrocarbons and a TCD detector by using a Porapack-Q column for inorganic materials.

[0053] The following examples are given by way of illustration of the working of the invention in actual practice and should not be construed to limit the scope of the present invention in any way.

Example 1

[0054] An aqueous solution of a given amount of silver nitrate (AgNO₃, 0.787 g) was added to vigorously stirred tungstic acid (H₂WO₄, 10.77 g) solution. The pH of the medium was made 9 by adding ammonium hydroxide solution. Then an aqueous solution of cetyltrimethyl ammonium bromide (CTAB, 1.26 g) was added to the mixture of two metal precursors. Finally, 0.28 g of aqueous solution of hydrazine was added drop wise. The reagents were added maintaining the following molar ratio:

Ag/CTAB/H₂O/hydrazine=1:0.75:3:0:1.

[0055] After stirring 4 hrs at room temperature (25°C) until a homogeneous solution was obtained, the resultant mixture was washed with ethanol, and dried at 110°C C., for 24 hours, followed by calcination at 650°C for 5 hrs.

[0056] The catalyst can be denoted as Ag₂O—WO₃ (5 wt% Ag, 75.4% W and 19.6 wt % O).

Example 2

[0057] An aqueous solution of a given amount of silver nitrate (AgNO₃, 1.574 g) was added to vigorously stirred tungstic acid (H₂WO₄, 10.77 g) solution. The pH of the medium was made 9 by adding ammonium hydroxide solution. Then an aqueous solution of cetyltrimethyl ammonium bromide (CTAB, 1.26 g) was added to the mixture of two metal precursors. Lastly, 0.28 g of aqueous solution of hydrazine was added drop wise. The reagents were added maintaining the following molar ratio:

Ag/CTAB/H₂O/hydrazine=1:0.75:3:0:1.

[0058] After stirring 4 hrs at room temperature (25°C) until a homogeneous solution was obtained, the resultant mixture was washed with ethanol, and dried at 130°C, for 24 hours, followed by calcination at 700°C for 4 hrs.

[0059] The catalyst can be denoted as Ag₂O—WO₃ (10 wt% Ag, 71.3% W and 18.7 wt % O).

Example 3

[0060] This example describes the epoxidation of propylene to propylene oxide by vapour phase reaction in presence of oxygen using Ag supported W-oxide as the catalyst.

Process Conditions

- Catalyst: Silver supported on tungsten oxide nanorod 0.3 g (catalyst prepared in Example 1 was used)
- Ag/W oxide weight ratio in the catalyst= 1:20
- Oxygen pressure = 3 Mpa
- Weight hourly space velocity (WHSV): 10000 h⁻¹
- Temperature: 375°C
- Reaction time: 6 h
- Product analysis:
  - Propylene conversion: 45%
  - Selectivity of propylene oxide: 100%
  - Yield of propylene oxide: 45%

Example 4

[0071] The example describes the effect of temperature on yield and selectivity of propylene oxide. The product analysis presented in Table 1.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Conversion (%)</th>
<th>Yield</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>15.8</td>
<td>15.8</td>
<td>100</td>
</tr>
<tr>
<td>250</td>
<td>20.3</td>
<td>20.3</td>
<td>100</td>
</tr>
<tr>
<td>300</td>
<td>24.6</td>
<td>24.6</td>
<td>100</td>
</tr>
<tr>
<td>350</td>
<td>36.3</td>
<td>36.3</td>
<td>100</td>
</tr>
<tr>
<td>400</td>
<td>47.3</td>
<td>47.3</td>
<td>97.1</td>
</tr>
</tbody>
</table>

Example 5

[0078] The example describes the effect of time on stream on yield and selectivity of propylene oxide. The product analysis presented in Table 2.

<table>
<thead>
<tr>
<th>Time on stream (h)</th>
<th>Propylene oxide yield and selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Conversion, %)</td>
</tr>
<tr>
<td>2</td>
<td>44.8</td>
</tr>
<tr>
<td>6</td>
<td>45.1</td>
</tr>
<tr>
<td>12</td>
<td>45.1</td>
</tr>
</tbody>
</table>

TABLE 1

Effect of temperature on propylene conversion, propylene oxide yield and selectivity.

TABLE 2

Effect of time on stream on propylene conversion, propylene oxide yield and selectivity.

195
TABLE 2-continued

<table>
<thead>
<tr>
<th>Time on stream (h)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield (%)</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>45.4</td>
<td>43.4</td>
<td>100</td>
</tr>
<tr>
<td>28</td>
<td>44.9</td>
<td>44.9</td>
<td>100</td>
</tr>
</tbody>
</table>

Example 6

The example describes the effect of oxygen pressure on yield and selectivity of propylene oxide. The product analysis presented in Table—3.

Process Conditions:

- Catalyst: Silver supported on tungsten oxide nanorod 0.3 g (catalyst prepared in Example 1 was used)
- Ag-W oxide weight ratio in the catalyst = 1:20
- Weight hourly space velocity (WHSV): 10000 h⁻¹
- Temperature: 375° C
- Reaction time: 6 h

Table 3

<table>
<thead>
<tr>
<th>Reaction Pressure (MPa)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield (%)</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>17.3</td>
<td>17.3</td>
<td>100</td>
</tr>
<tr>
<td>3</td>
<td>45.0</td>
<td>45</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>46.1</td>
<td>43.8</td>
<td>95.1</td>
</tr>
<tr>
<td>5</td>
<td>47.3</td>
<td>39.9</td>
<td>84.3</td>
</tr>
</tbody>
</table>

Example 7

The example describes the effect of weight hourly space velocity on yield and selectivity of propylene oxide. The product analysis presented in Table—4.

Process Conditions:

- Catalyst: Silver supported on tungsten oxide nanorod 0.3 g (catalyst prepared in Example 1 was used)
- Ag-W oxide weight ratio in the catalyst = 1:20
- Oxygen pressure: 3 MPa
- Temperature: 375° C
- Reaction time: 6 h

Table 4

<table>
<thead>
<tr>
<th>WHSV (ml feed/kg-cat)</th>
<th>Propylene Conversion (%)</th>
<th>Propylene Oxide Yield (%)</th>
<th>Selectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>49.1</td>
<td>44.9</td>
<td>91.4</td>
</tr>
<tr>
<td>4000</td>
<td>46.6</td>
<td>44.8</td>
<td>96.2</td>
</tr>
<tr>
<td>6000</td>
<td>45.0</td>
<td>45</td>
<td>100</td>
</tr>
<tr>
<td>20000</td>
<td>35.1</td>
<td>35.1</td>
<td>100</td>
</tr>
</tbody>
</table>

The main advantages of the present invention are:

1. The process of the present invention converts propylene to propylene oxide in a single step with a single catalyst.
2. The process provides not only good conversion but also good selectivity for propylene oxide.
3. The oxidizing agent, oxygen, used in this process has the major advantages of this process.
4. The process does not produce any by-products also is a major advantage of this process.
5. The catalyst is used in very low amounts.
6. The process does not need any additional reagent to generate active oxygen.
7. The catalyst does not deactivate till 30 h with the reaction stream.

1. A process for the preparation of Ag-W oxide catalyst, said process comprising the steps of:
   a. mixing a salt of Ag, WO₃, H₂O, a surfactant, a reducing agent hydrate and H₂O to obtain a gel;
   b. mixing gel as obtained in step (a) with constant stirring for 2-6 h at room temperature ranging between 25-35° C;
   c. filtering the gel as obtained in step (b) and washing with excess water and dried in an oven with temperature ranging between 100-120° C for a period ranging between 6-18 hours;
   d. calcining the dried product as obtained in step (c) at temperature ranging between 300-750° C for a period ranging between 4-10 h to obtain Ag-W oxide catalyst.
2. The process as claimed in claim 1, wherein weight ratio of Ag to W in step (a) is in the range of 0.05 to 0.5.
3. The process as claimed in claim 1, wherein molar ratio of Ag to CTAAB in step (a) is in the range of 0.75-1.3.
4. The process as claimed in claim 1, wherein molar ratio of Ag to hydrate in step (a) is in the range of 0.75-1.3.
5. A single step process for selective oxidation (epoxidation) of propylene to propylene oxide using Ag-W oxide catalyst as obtained by the process as claimed in claim 1, wherein the said process comprising the steps of reacting propylene with oxygen in the presence of Ag-W oxide catalyst in the pressure range of 1—5 Mpa, at a temperature ranging between 150-450° C with a weight hourly space velocity (WHSV, feed/g catalyst/hour) in the range of 2000 to 500001 h⁻¹ for a period in the range of 1-20 hours to obtain propylene oxide.
6. The process as claimed in claim 5, wherein the conversion of propylene oxide is in the range of 10-50%.
7. The process as claimed in claim 5, wherein the selectivity of the propylene oxide obtained in the range of 80-100%.
8. The process as claimed in claim 5, wherein the yield of propelene oxide is in the range of 10-50%.
9. The process as claimed in claim 1, wherein the salt of Ag comprises AgNO₃.
10. The process as claimed in claim 1, wherein the surfactant comprises cetyltrimethylammonium bromide (CTAB).