Propane to Acrylic Acid

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April 9, 2013

Advisor: Dr. John Vohs

Primary Consultant: Bruce M. Vrana

University of Pennsylvania
Department of Chemical and Biomolecular Engineering
220 South 33rd Street
Philadelphia, PA 19104

April 9th, 2013

Dear Dr. Vohs and Professor Fabiano,

Enclosed you will find the proposed process design for the industrial production of acrylic acid as a solution to the design problem presented by Bruce Vrana of DuPont. The proposed design uses a mixed metal oxide catalyst, $Mo_1V_{0.30}Te_{0.23}Nb_{0.125}O_x$, in a fixed bed reactor to selectively oxidize propane to acrylic acid using propylene and acrolein inermediates**.** The product is separated using a flash distillation column from leftover starting materials, which are recycled back to the reactor. Then, the acrylic acid is purified from water, acetic acid, and trace amounts of unreacted materials using four distillation towers. The proposed plant will be constructed in the U.S. Gulf Coast and will produce 200 MM lb/year of industrial-grade acrylic acid.

This report contains a detailed process design, an economic analysis, and conclusions and recommendations for the implementation of the plant. The proposed process is found to be viable and economically profitable with an estimated IRR of 84.9% with a total NPV of $384,963,400 at a discount rate of 15%**.** The process was modeled using AspenTech Plus v7.3. Economic analysis and equipment sizing was conducted using Aspen IPE and Aspen Economic Evaluation v7.3 along with the equations spreadsheets contained in *Process Design Principles*, 3rd Edition, by Seider, Seader, Lewin and Widagdo.

Thank you for your assistance with this project.

Sincerely,

Amanda Culp	Kevin Holmes
Rohan Nagrath	Dan Nessenson

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Section 1

Abstract

Abstract

Acrylic acid is an essential polymer raw material for many industrial and consumer products. Currently, acrylic acid is manufactured from propylene, which is created as a by-product from fossil fuels manufacture and industrial cracking of heavy hydrocarbons. However, the discovery of new natural gas reserves presents new opportunities for the production of acrylic acid. A design feasibility study is presented to analyze the economics behind producing acrylic acid from the selective oxidation of propane to propylene over a mixed metal oxide catalyst, $Mo_1V_{0.30}Te_{0.23}Nb_{0.125}O_x$.

The proposed plant is located in the U.S. Gulf Coast and produces 200MM lb/yr acrylic acid. Since the catalytic oxidation process has low propane conversion per pass, the process recycles unconverted propane and propylene back to the reactor to increase overall conversion. The acrylic acid is then separated and purified to the glacial-grade industrial standard for polymer raw material of 99.7% acrylic acid by mass. A major challenge of the separation process is the non-ideal behavior of the components, which produces three different azeotropes: water with acrylic acid, water with acetic acid, and acetic acid with acrylic acid. The separation process utilizes four distillation towers to navigate around the azeotropes.

After a thorough economic analysis, the proposed process is found to be economically viable. It has an estimated IRR of 84.9% and NPV of $384,963,400 at a 15% discount rate using an acrylic acid price of $1.75/lb. The process is predicted to become profitable in year 3. If the product price decreases by 45% to $1.20/lb (the current market price of acrylic acid), the estimated IRR will be 45% with a NPV of $114,552,700 at a 15% discount rate. The process will then become profitable in year 4.

Section 2

Introduction and Background Information

2.1 Introduction and Background Information

Acrylic acid is essential for the production of many consumer and industrial products. Two grades of acrylic acid are commercially available: technical-grade and glacial-grade. Technical, or crude, acrylic acid is approximately 94% purity by mass and is synthesized to acrylate esters. The esters are converted to co-monomers which, when polymerized, are used to make surface coatings, adhesives, sealants, textiles, and paints. Acrylate esters have many desirable qualities for polymeric materials such as color stability, heat and aging resistance, weather durability, low temperature flexibility, and resistance to acid and bases.[1] Glacial, or industrial, acrylic acid is generally 99.5% to 99.7% acrylic acid by mass and is polymerized to produce polyacrylic acid-based polymers.[2] These polymers are used to make detergents, dispersants, super absorbent polymers (such as in diapers), and thickeners. The breakdown of U.S. acrylic acid consumption by end-use is displayed in Figure 2.1**:**

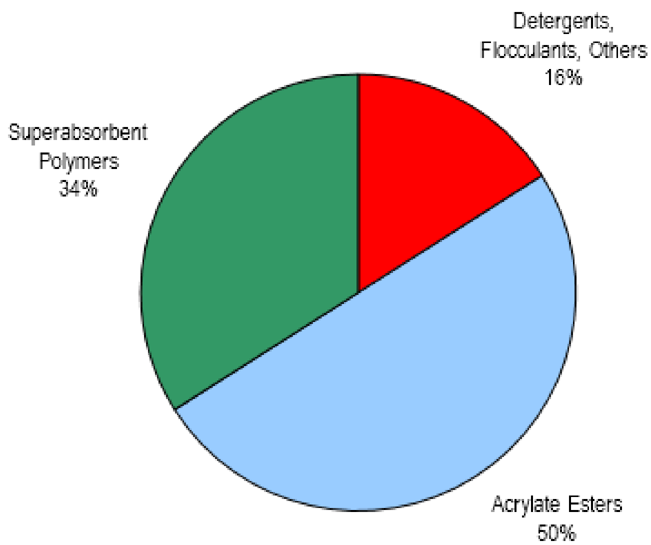

Figure 2.1: U.S. Acrylic Acid by End-Use[2]

Acrylic acid is typically produced through a two-stage propylene-based oxidation process using acrolein as a fast-acting intermediate, as depicted below:

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[1] ICIS Chemical Business (2010). Acrylic Acid Uses and Market Data. Retrieved March 31, 2013, from

[2] Nexant, Inc. (2010). Acrylic Acid. Retrieved March 31, 2013, from http://www.chemsystems.com/reports/search/docs/abstracts/0809_3_abs.pdf

$$H_2C = CHCH_3 + O_2 \rightarrow H_2C = CHCHO + H_2O \quad (1)$$

$$\Delta H = -340\ kJ/mol$$

$$H_2C = CHCHO + 0.5O_2 \rightarrow H_2C = CHCOOH \quad (2)$$

$$\Delta H = -254.1\ kJ/mol$$

Overall selectivities of 80% to 90% of acrylic acid based on propylene are obtained at conversions over 95%. However, there is room for optimization in this process by using a cheaper starting material, such as propane.

Hydraulic fracturing, commonly referred to as fracking, is a technique used to release petroleum and natural gas in a rock layer deep below the earth's surface using a pressurized fluid. At such depth, natural gas and oil do not have enough reservoir pressure to flow at economically desirable rates from the well or bed. Creating fractures in the rock increases the permeability of the reservoir. Although there is controversy over the environmental impacts, these effects can be mitigated through best practices and strict legislation. As of 2010, it is estimated that 60% of all new oil and gas wells were hydraulically fractured.[3] Fracking has a large economic impact because of its ability to extract vast amounts of formerly inaccessible hydrocarbons. As a result, prices for hydrocarbon liquids have fallen significantly. This development has made it economically advantageous to use propane as a starting material for acrylic acid production using the pathway described in U.S. Patent 8,193,387.

Producing an unsaturated acid, such as acrylic acid, from a saturated hydrocarbon has previously been difficult with the notable exception of butane to maleic anhydride. However, recent advancements in mixed metal oxide catalysts have created a process to convert propane to acrylic acid in high yield. This report investigates this process by first oxidizing propane to propylene and then implementing a two-stage propylene-based oxidation process as previously discussed. The oxidation reactions are highly exothermic and are performed in the presence of a mixed metal oxide catalyst in a fixed-bed reactor using a Dowtherm cooling system. The overall goal of this design process is to produce a plant which will yield 200 MM lb/year glacial-grade acrylic acid.

[3] Montgomery, C. T., & Smith, M. B. (2010). Hydraulic Fracturing: History of an Enduring Technology. Retrieved March 31, 2013, from http://www.spe.org

2.2 Project Charter

Project Name: Propane to Acrylic Acid

Project Consultants: Bruce M. Vrana (DuPont)
Dr. John Vohs (UPenn)
Professor Leonard Fabiano (UPenn)

Project Leaders: Amanda Culp
Kevin Holmes
Rohan Nagrath
Dan Nessenson

Specific Goals: Design and determine the economic viability of a plant that produces competitive amounts of industrial-grade acrylic acid through oxidation of propane via a mixed metal oxide catalyst in a fixed bed reactor.

Project Scope:

In Scope:

- Selecting an optimal mixed metal oxide catalyst
- Estimating reaction kinetics of propane to acrylic acid via propylene intermediate
- Creating a process design of a plant that produces 200 MM lb/yr acrylic acid
- Completing approximate equipment sizing
- Determining economic viability of the proposed plant
- Determining profitability of the project if deemed to be economically viable

Out of scope:

- Verifying reaction kinetics, conversions, and yields proposed in literature
- Developing wastewater treatment facilities
- Determining safety layout of facilities

Deliverables:

- Full Plant Design
- Detailed Economic Analysis
- Approximate Equipment Sizing

Timeline:

- Initial process design completed by February 19th, 2013
- Initial equipment sizing completed by March 12th , 2013
- Initial economic analysis completed by March 26th, 2013
- Deliverables completed by April 9th, 2013

2.3 Technology-Readiness Assessment

The motivation behind this process design is driven by both advancements in technology and an increase in market size. Technologically driven aspects of the process include (1) the use of a mixed metal oxide catalyst, $Mo_1V_{0.30}Te_{0.23}Nb_{0.125}O_x$, (2) the use of a recycle stream to increase the yield of acrylic acid while keeping selectivity high and per pass propane conversion low, and (3) the use of hydraulic fracturing to produce a cheap starting material, propane. All of these technologies are currently available for use and can be readily implemented. The Innovation Map for this process is shown in Figure 2.2, page 8.

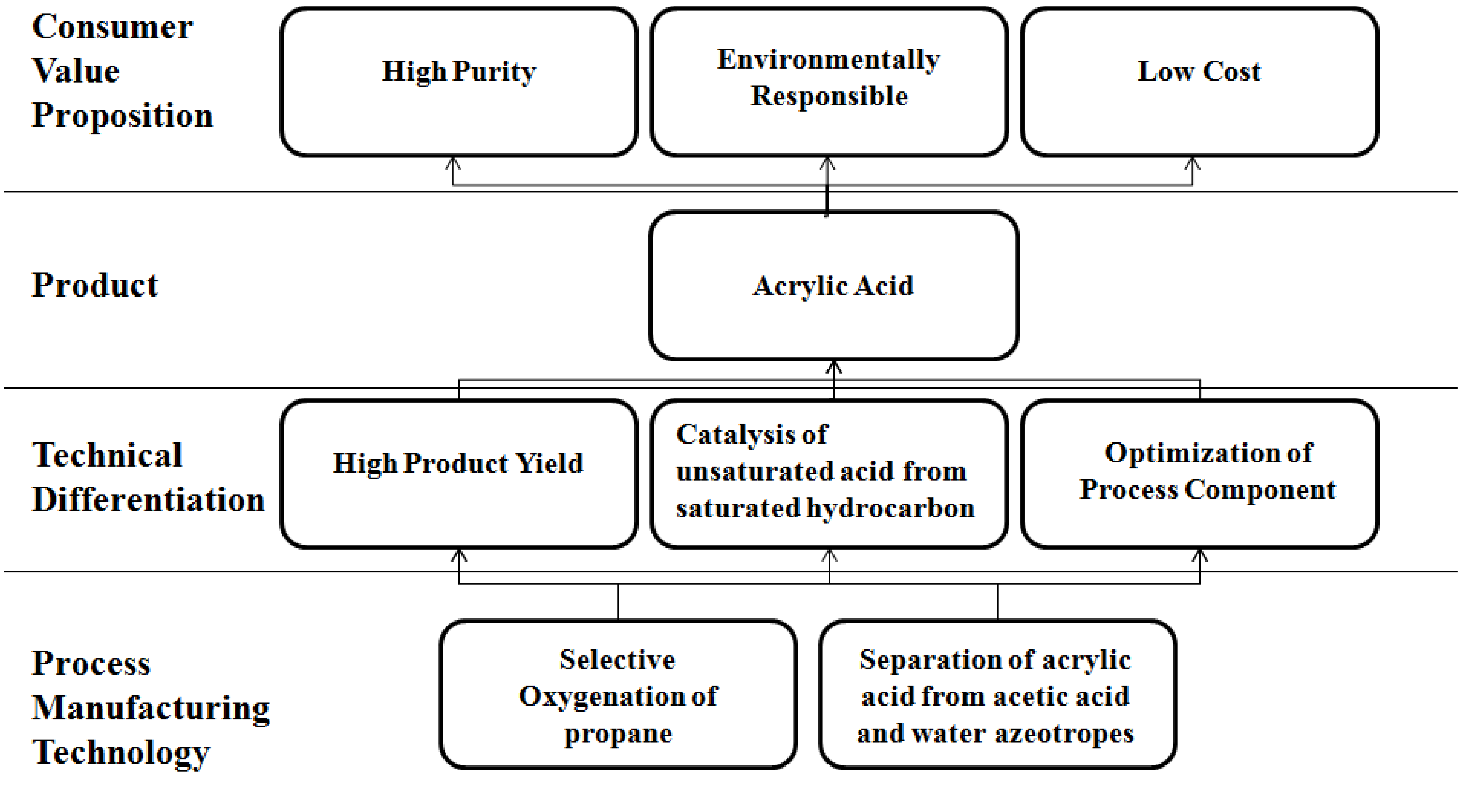

Figure 2.2: Innovation Map

Section 3

Concept Stage

3.1 Market and Competitive Analysis

Due to acrylic acid's use in a number of consumer and industrial applications (including adhesives, paints, plastics, hygiene products, and detergents), there exists an $11 billion market for the compound. The growth in Western Europe and the United States has slowed down to around 1.6% per year. However, because China and India have begun to adopt U.S. production techniques and strategies, the need for polymers and copolymers has increased, adding to the growing demand for acrylic acid. China, in particular, is the high-growth market for acrylic acid and is increasing its consumption by approximately 8% per year.[4] The average world demand is growing at a rate of approximately 3% to 5% per year. Worldwide, the acrylic acid market is predicted to be worth $14 billion by 2018.

Because this proposed process uses a cheaper raw material and produces a higher yield of acrylic acid at the same purity, it should be competitive within the existing industrial market. However, the proposed acrylic acid plant may face a number of competitive challenges from renewable acrylic acid pathways. The selling price of acrylic acid is predicted to drop if bio-acrylic acid plants are able to scale-up their process to industrial production levels. OPX Biotechnologies, a leader in the fermentation process used to produce acrylic acid, is able to produce a $0.50/lb acrylic acid which is much cheaper than the price of acrylic acid ($1.75/lb) which was assumed in this project.[5]

[4] ICIS Chemical Business (2010). Acrylic Acid Uses and Market Data. Retrieved March 31, 2013, from http://www.icis.com/Articles/2007/11/01/9074870/acrylic-acid-uses-and-market-data.html

[5] Guzman, D. d. (2012). Bio-acrylic acid on the way. Retrieved March 31, 2013, from http://greenchemicalsblog.com/2012/09/01/5060/

3.2 Customer Requirements

Customer requirements for this process are standardized due to the high demand in the existing market. There are two grades of acrylic acid which are commercially available. Glacial, or industrial-grade, which is 99.7% acrylic acid by mass, is used for the production of super absorbent polymers for water treatment, disposable diapers, and detergents. Technical-grade, or crude acrylic acid, which is approximately 94% acrylic acid by mass, is mostly used for the production of surface coatings, adhesives, plastic additives, and paper treatment. Customer requirements for this process are based on the existing industry market standard for glacial-grade acrylic acid.

Typically acrylic acid is stored as a purified liquid, immediately after production, and pumped when sold. Acrylic acid and related acrylate esters polymerize in the presence of heat, light, and peroxides. Thus, stabilizers such as hydroquinone or the monomethyl ether of hydroquinone (MEHQ) must be added in the presence of oxygen to inhibit polymerization and prolong shelf life.[6] Storage and shipment temperatures should be kept in the range of 59°F to 77°F and under atmospheric pressure with air to prevent undesired reactions. Acrylic acid should not be stored with any inert gases so as to prevent premature polymerization. Because acrylic acid is corrosive, it must be shipped in stainless steel, aluminum, or polyethylene drums. Safety requirements demand that the containers are labeled as corrosive, flammable, and dangerous to the environment.

[6] BASF Corporation (2007). Acrylic Acid: A Summary of Safety and Handling. http://msdssearch.dow.com/PublishedLiteratureDOWCOM/dh_0042/0901b80380042934.pdf?filepath=acrylates/pdfs/noreg/745-00006.pdf&fromPage=GetDoc (p8)

3.3 Preliminary Process Synthesis

Acrylic acid is typically produced through the catalytic partial oxidation of propylene:

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O \quad (3)$$

Additionally, acrylic acid can also be produced through a one-step selective oxidation of propane over a selective catalyst:

$$C_3H_8 + 2O_2 \rightarrow C_3H_4O_2 + 2H_2O \quad (4)$$

The proposed reaction network is displayed in Figure 3.1 (below) with the activation energies of the pathways shown and the asterisks indicating active intermediates.[7] It is believed that propylene may pass through an σ-allyl radical intermediate before it reaches acrolein as displayed in red below.[8]

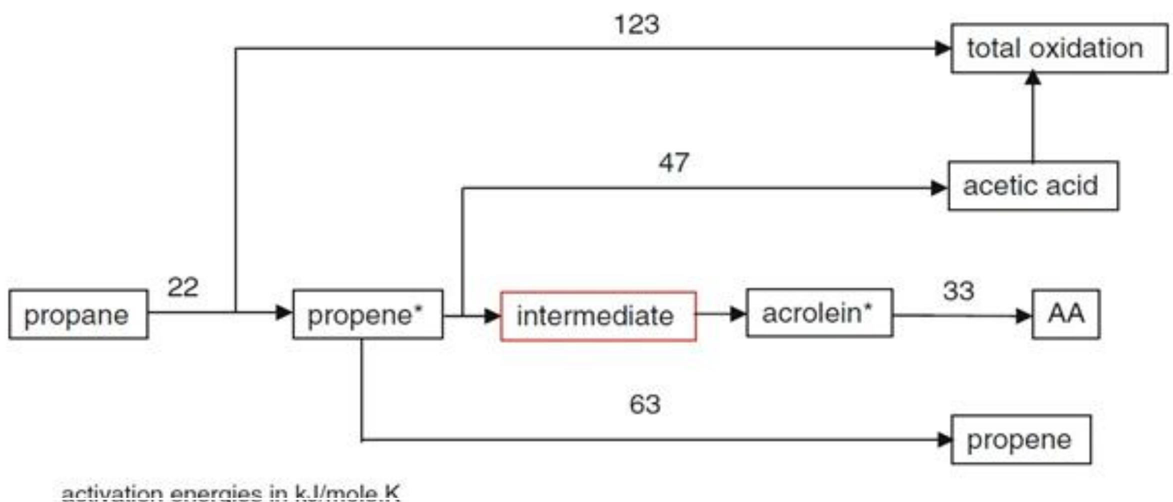

Figure 3.1: Proposed Oxidation Pathway on Diluted Mo-V-Te-Nb Mixed Oxide Catalyst

Side reactions of this process include total oxidation as seen in reactions (5)-(7) and the production of acetic acid through activated propylene or acrolein in reaction (8). The total oxidation side reactions can be minimized by maintaining the reactor temperature at the desired level by removing excess heat from the highly exothermic reaction. Additionally, the use of an

[7] Widi, R. K., Hamid, S. B. A., & Schlogl, R. (2009). Kinetic investigation of propane oxidation on diluted Mo1-V0.3-Te0.23-Nb0.125-Ox mixed-oxide catalysts. Reaction Kinetics and Catalysis Letters, 98, 273-286.
[8] Pudar, S., Oxgaard, J., Chenoweth, K., van Duin, A., & Goddard, W. (2007). Mechanism of Selective Oxidation of Propene to Acrolein on Bismuth Molybdates from Quantum Mechanical Calculations. Materials and Process Simulation Center, 111, 16405-16415. http://www.wag.caltech.edu/home/ch120/Lectures/Pudar2007.pdf

inert gas, such as water or nitrogen, may prevent excess oxidation of propylene by enhancing the desorption of acrylic and acetic acids from the catalyst surface.

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \quad (5)$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O \quad (6)$$

$$C_2H_4O_2 + 2O_2 \rightarrow 2CO_2 + 2H_2O \quad (7)$$

$$C_3H_4O + \frac{3}{2}O_2 \rightarrow CO_2 + C_2H_4O_2 \quad (8)$$

Kinetics

Propane partial oxidation to acrylic acid over vanadium pyrophosphate (VPO) catalysts, heteropolyacids, and multi-component oxidic catalysts has been studied in great depth. Only recently has a catalyst system been developed that is active and selective enough to substitute for the existing industrial process.[9] This is due to the difficulty in maintaining high reaction temperatures (so the reaction rate will be high) while preventing total oxidation reactions. A thorough review of mixed metal oxide catalyst literature was performed and the results are summarized in Table 3.1.[10] The conversions listed are based on propane and the yield and selectivities are based on acrylic acid.

Table 3.1: Mixed metal-oxide Catalysts for Propane Oxidation to Acrylic Acid

Catalyst	**Feed**	Temp (^oC)	Conversion (%)	Yield (%)	Selectivity (%)
$Mo_1V_{0.3}Nb_{0.05}Sb_{0.15}Te_{0.06}O_x$	Propane/O_2/H_2O/N_2	380	21	12	54
$Mo_1V_{0.3}Nb_{0.05}Sb_{0.09}Te_{0.09}O_x$	Propane/O_2/H_2O/N_2	380	19	12	60
$Mo_1V_{0.3}Sb_{0.16}Nb_{0.05}O_x$	Propane/air/ H_2O	380	50	16	32
$Mo_1V_{0.3}Sb_{0.25}Nb_{0.11}O_x$	Propane/O_2/H_2O/N_2	400	21	12	61
$Mo_1V_{0.3}Te_{0.23}Nb_{0.125}O_x$	Propane/air/H_2O	400	80	48	60
$Mo_1V_{0.3}Te_{0.23}Nb_{0.12}O_x$	Propane/air/H_2O	390	71	42	59
$Mo_1V_{0.3}Te_{0.23}Nb_{0.12}O_x$	Propane/O_2/H_2O/He	350	23	14	61

According to experimental data, the most effective catalysts to date are Mo-V-Te-Nb-O catalysts. The proposed process design uses the $Mo_1V_{0.3}Te_{0.23}Nb_{0.125}O_x$ catalyst.

[9] Hatano, M. & Kayo, A. (1991). U.S. Patent No. 5,049,692.
[10] Lin, M. (2001). Selective oxidation of propane to acrylic acid with molecular oxygen. Applied Catalysis A: General, 207, 1-16.

Separation

After acrylic acid is produced, it must be separated from the reactants (oxygen, nitrogen, and propane) and the by-products of the reaction (acetic acid, water, and propylene). While a simple flash drum will be able to separate the reactants from acrylic acid, the final product separation from acetic acid and water is difficult due to three separate azeotropes as seen in Figure 3.2:

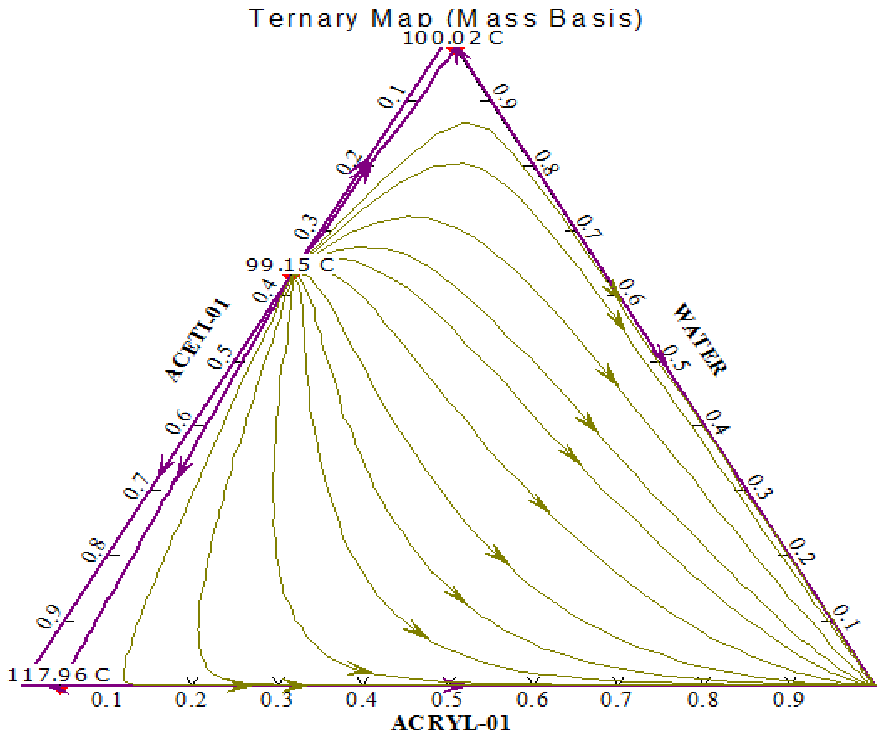

Figure 3.2: Azeotrope Diagram for Acetic Acid/Water/Acrylic Acid. The diagram was produced using Aspen, based on the NRTL-RK model.

In order to determine the most economic and efficient method of separation, three different processes were evaluated and the results compared. The first proposed method of separation, displayed in Figure B.2 (located in Appendix B, page 133), involved the use of a liquid-liquid extraction process to allow better separation of organic components from water. The product stream from the reactor was fed to a flash drum and a distillation column, which separated and recycled the gaseous components. The bottoms product was separated in an eight-tray column into a pure acrylic acid stream. The distillate contained water, acetic acid, and residual acrylic acid and was fed into a decanter. The decanter was operated with n-propyl acetate, an extraction solvent recommended by U.S. Patent Number 5,315,037.[11] The decanter succeeded in separating the mixture into a water stream containing 97% by mass water and the balance organic components and an organic stream. Through a series of two more distillation columns a majority of the solvent (which can be recycled), and 96% of the total acrylic acid were recovered. Ultimately, this method of separation was not selected because the additional costs associated with the decanter and the solvent feed of n-propyl acetate did not result in better acrylic acid separation.

The second method of separation proposed was an extractive distillation process performed in a distillation column, which eliminated the use of a decanter but still required an entrainer.[12] An Aspen diagram of the separation process can be seen in Figure B.3 (located in Appendix B, page 134). The extractive agent is introduced near the top of the column and its presence alters the relative volatility of the compounds to allow a greater degree of separation. After a separation using different entrainers (based on suggestions from U.S. Patent 5,154,800[12]) was designed in Aspen, dimethylsulfoxide was selected as the optimal extractive agent. As with the decanter process, this method of separation was not selected because it did not result in higher acrylic acid separation despite the added cost of solvent and keeping the number of distillation towers (four) used the same.

The final separation process evaluated was a network of four distillation towers which maneuvered around the azeotropes within the system. This processes proved to be better than the other two alternatives based on cost, optimal separation of acrylic acid and final stream purity. This separation scheme is discussed later on in detail.

[11] Sakamoto, K., Tanaka, H., Ueoka, M., Akazawa, Y., & Baba, M. (1994). U.S. Patent No. 5,315,037.

[12] Berg, L. (1992). U.S. Patent No. 5,154,800.

3.4 Assembly of Database

Input Costs

The input cost for water, including pressurized steam, was taken from Aspen Economic Analyzer. Current pricing from Aspen is based on 2010 dollars, so a multiplying factor of 1.0447 (CE 2012/2010 = 575.4/550.8) was used. Input costs for liquid propane and compressed oxygen were specified in the problem statement found in Appendix A, page 130.

Aspen Simulation Specifications

In this project, Aspen Plus v7.3 was used. All simulations should be run in this version of Aspen to avoid compatibility issues. In order to accurately model the three azeotropes in the process, the non-random two-liquid (NRTL) activity coefficient model, along with the Redlich-Kwong (RK) equation of state model, was used in all simulations. RStoic was used over a PFR model reactor, as conversion, selectivities, and yield data was more easily available and more complete than kinetic models (which are needed for PFR models in Aspen). RStoic was used to model the conversion information taken from patented processes, and to model the heat rise in the reactor with given conversion data. MComp was used to model the two compressor blocks in the system. The compressors were designed to have the lowest possible outlet pressure conditions such that pressure conditions into the Flash block were as specified without doing extra work. Heat exchangers, including the reactor, were designed outside of Aspen.

Design specifications were used to optimize conditions in the system. Design specifications were used to change reflux ratio and distillate-to-feed ratio in each tower to ensure the purity of acrylic acid. Tower trays and feed location were optimized by plotting tray temperatures and tray concentrations to eliminating dead zones. A design specification for the oxygen inlet flow rate was used such that propane exiting the reactor was in extreme excess of oxygen (so that further oxidation is limited).

Section 4

Process Flow Diagram & Material Balance

4.1 Overall Process Outline

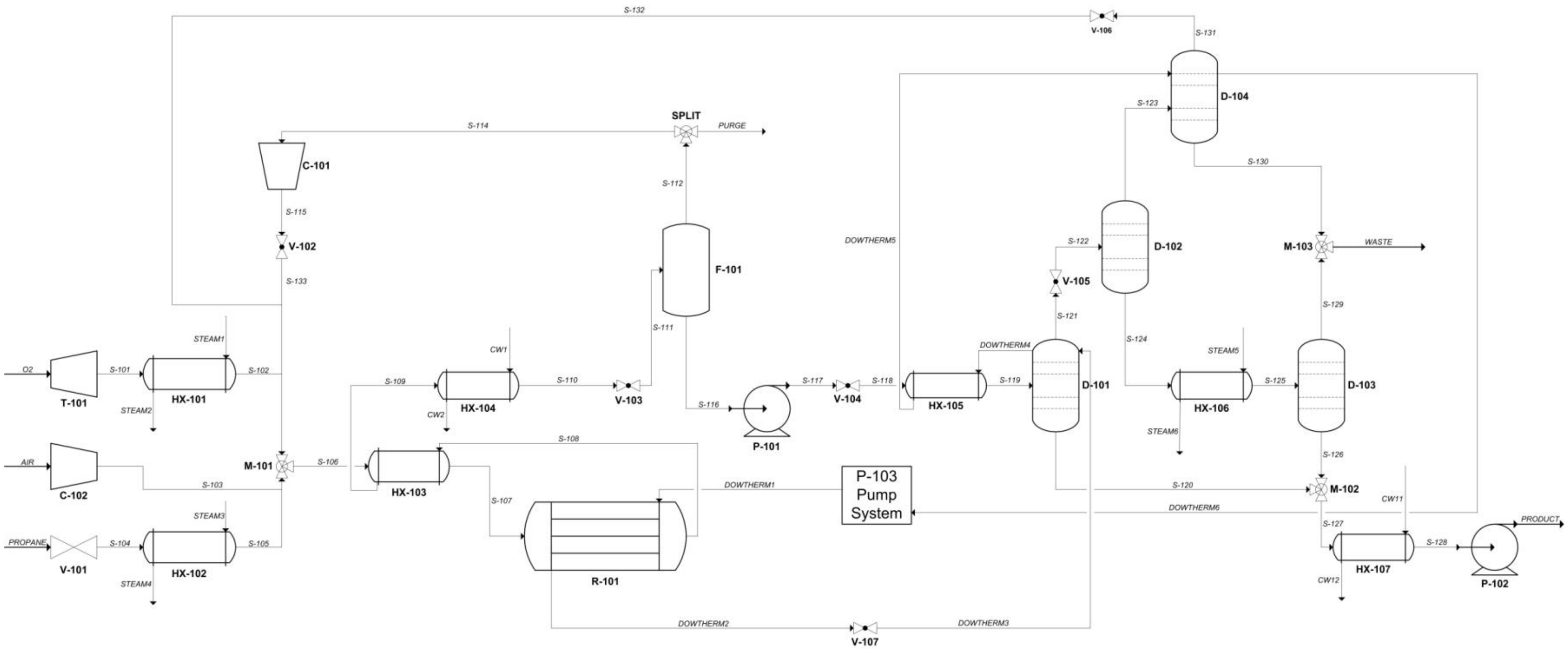

Figure 4.1: Overall Process Diagram. This shows the overall process, which is made up of three sections: the mixing section, the reactor section, and the separation section.

Table 4.1: Overall Process Stream Summary. This table provides temperature, pressure, vapor fraction, and component flow rates for all streams in the process flowsheet.

Stream	S-133	AIR	O2	PRODUCT	PROPANE	PURGE	S-101	S-102	S-103	S-104	S-105	S-106	S-107	S-108	S-109	S-110	S-111	S-112	S-114
Temperature (°F)	225	75	75	100	75	85	-106	230	406	24	230	228	740	780	280	85	82	85	85
Pressure (psia)	54	14.6959	500	75	150	25	60	55	54	60	55	54	49	45	40	35	30	25	25
Vapor Fraction	1	1	1	0	0	1	1	1	1	0.2	1	1	1	1	1	0.92	0.92	1	1
Total Flow (lb/hr)	554490	12636	23839	25314	23616	17149	23839	23839	12636	23616	23616	620230	620230	620230	620230	620230	620230	571630	554490
Component Flows (lb/hr)																			
Propane	153820	0	0	0	23616	4757	0	0	0	23616	23616	180250	180250	162230	162230	162230	162230	158570	153820
Oxygen	2427	2943	23839	0	0	75	23839	23839	2943	0	0	29212	29212	2505	2505	2505	2505	2502	2427
Propylene	19146	0	0	0	0	592	0	0	0	0	0	19451	19451	20119	20119	20119	20119	19739	19146
Acrylic Acid	1791	0	0	25286	0	55	0	0	0	0	0	1901	1901	28548	28548	28548	28548	1846	1791
Water	5713	0	0	25	0	177	0	0	0	0	0	7547	7547	22309	22309	22309	22309	5890	5713
Nitrogen	313410	9693	0	0	0	9693	0	0	9693	0	0	323240	323240	323240	323240	323240	323240	323110	313410
Acetic Acid	379	0	0	2.5	0	12	0	0	0	0	0	537	537	1393	1393	1393	1393	390	379
Carbon Dioxide	57798	0	0	0	0	1788	0	0	0	0	0	58094	58094	59894	59894	59894	59894	59585	57798
Dowtherm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Stream	S-115	S-116	S-117	S-118	S-119	S-120	S-121	S-122	S-123	S-124	S-125	S-126	S-127	S-128	S-129	S-130	S-131	S-132	WASTE
Temperature (°F)	225	85	86	86	400	418	318	317	295	307	374	371	415	100	298	287	265	264	236
Pressure (psia)	59	25	150	130	125	98	95	90	70	73	68	68	68	63	65	67	65	60	25
Vapor Fraction	1	0	0	0	1	0	1	1	1	0	1	0	0	1	1	0	1	1	0.3
Total Flow (lb/hr)	554490	48596	48596	48596	48596	23846	24750	24750	19472	5278	5278	1469	25314	25314	3809	13819	5653	5653	17628
Component Flows (lb/hr)																			
Propane	153820	3651	3651	3651	3651	0	3651	3651	3651	0	0	0	0	0	0	834	2817	2817	834
Oxygen	2427	3	3	3	3	0	3	3	3	0	0	0	0	0	0	0	3	3	0
Propylene	19146	380	380	380	380	0	380	380	380	0	0	0	0	0	0	75	305	305	75
Acrylic Acid	1791	26702	26702	26702	26702	23844	2858	2858	1024	1834	1834	1443	25286	25286	392	913	110	110	1305
Water	5713	16419	16419	16419	16419	0	16419	16419	13036	3383	3383	25	25	25	3358	11202	1834	1834	14560
Nitrogen	313410	130	130	130	130	0	130	130	130	0	0	0	0	0	0	0	130	130	0
Acetic Acid	379	1003	1003	1003	1003	1	1001	1001	941	60	60	1	3	3	59	783	158	158	842
Carbon Dioxide	57798	308	308	308	308	0	308	308	308	0	0	0	0	0	0	12	296	296	12
Dowtherm	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Stream	DOWTHERM-1	DOWTHERM-2	DOWTHERM-3	DOWTHERM-4	DOWTHERM-5	DOWTHERM-6
Temperature (°F)	198	738	458	299	203	198
Pressure (psia)	40	35	30	25	20	15
Vapor Fraction	0	0	0	0	0	0
Total Flow (lb/hr)	385000	385000	385000	385000	385000	385000
Component Flows (lb/hr)						
Dowtherm	385000	385000	385000	385000	385000	385000

4.2 Mixing Section

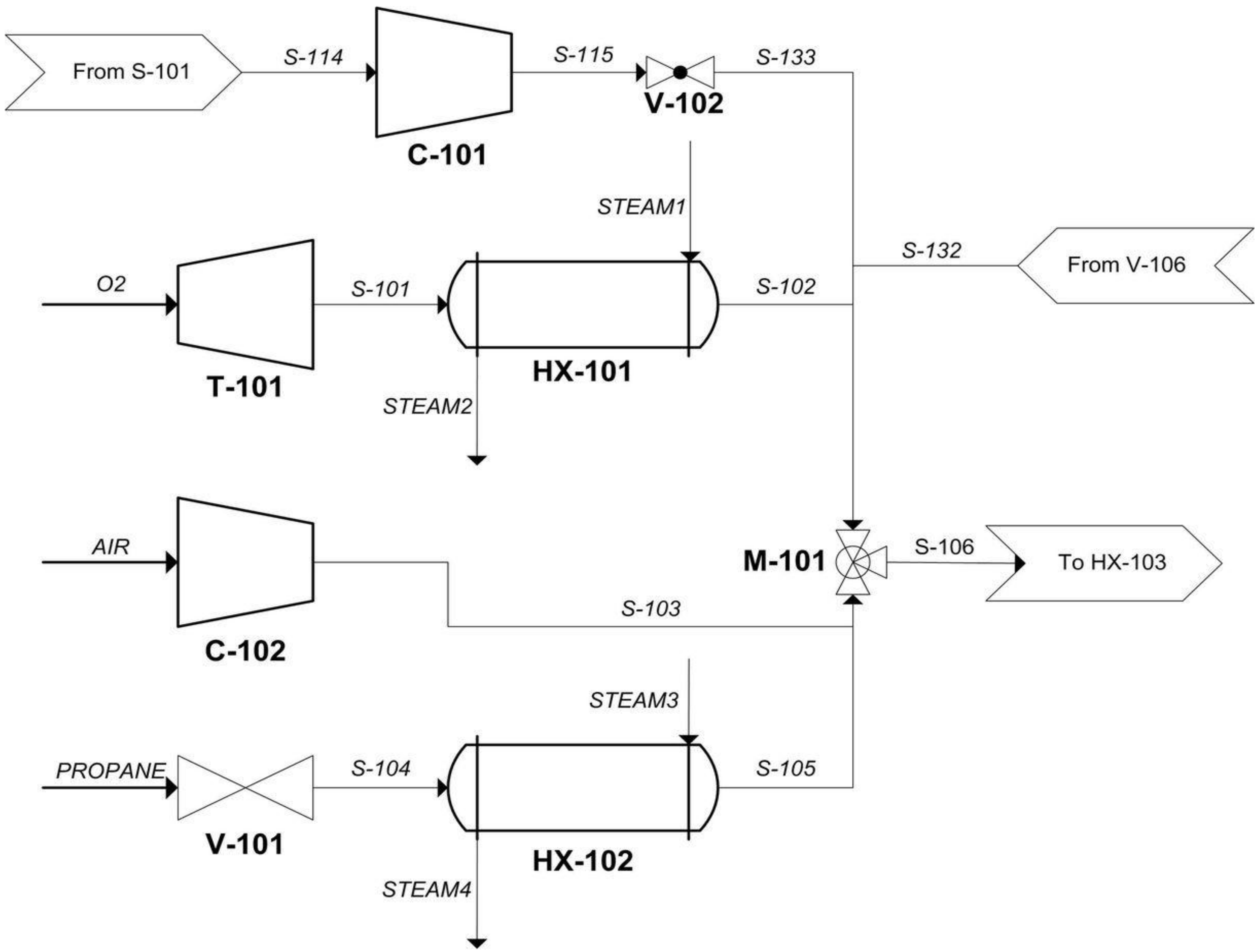

Figure 4.2: Mixing Section Process Diagram. This shows the flowsheet for the mixing section of the process.

Table 4.2: Mixing Section Stream Summary. This table provides temperature, pressure, vapor fraction, and component flow rates for all streams in the mixing section of the process flowsheet.

Stream	**S-114**	**S-115**	**S-133**	**O2**	**S-101**	**S-102**	**AIR**	**S-103**	**PROPANE**	**S-104**	**S-105**	**S-132**	**S-106**
Temperature (°F)	85	225	225	75	-106	230	75	406	75	24	230	264	228
Pressure (psia)	25	59	54	500	60	55	14.6959	54	150	60	55	60	54
Vapor Fraction	1	1	1	1	1	1	1	1	0	0.2	1	1	1
Total Flow (lb/hr)	554490	554490	554490	23839	23839	23839	12636	12636	23616	23616	23616	5653	620230
Component Flows (lb/hr)													
Propane	153820	153820	153820	0	0	0	0	0	23616	23616	23616	2817	180250
Oxygen	2427	2427	2427	23839	23839	23839	2943	2943	0	0	0	3	29212
Propylene	19146	19146	19146	0	0	0	0	0	0	0	0	305	19451
Acrylic Acid	1791	1791	1791	0	0	0	0	0	0	0	0	110	1901
Water	5713	5713	5713	0	0	0	0	0	0	0	0	1834	7547
Nitrogen	313410	313410	313410	0	0	0	9693	9693	0	0	0	130	323240
Acetic Acid	379	379	379	0	0	0	0	0	0	0	0	158	537
Carbon Dioxide	57798	57798	57798	0	0	0	0	0	0	0	0	296	58094
Dowtherm	0	0	0	0	0	0	0	0	0	0	0	0	0

4.3 Reactor Section

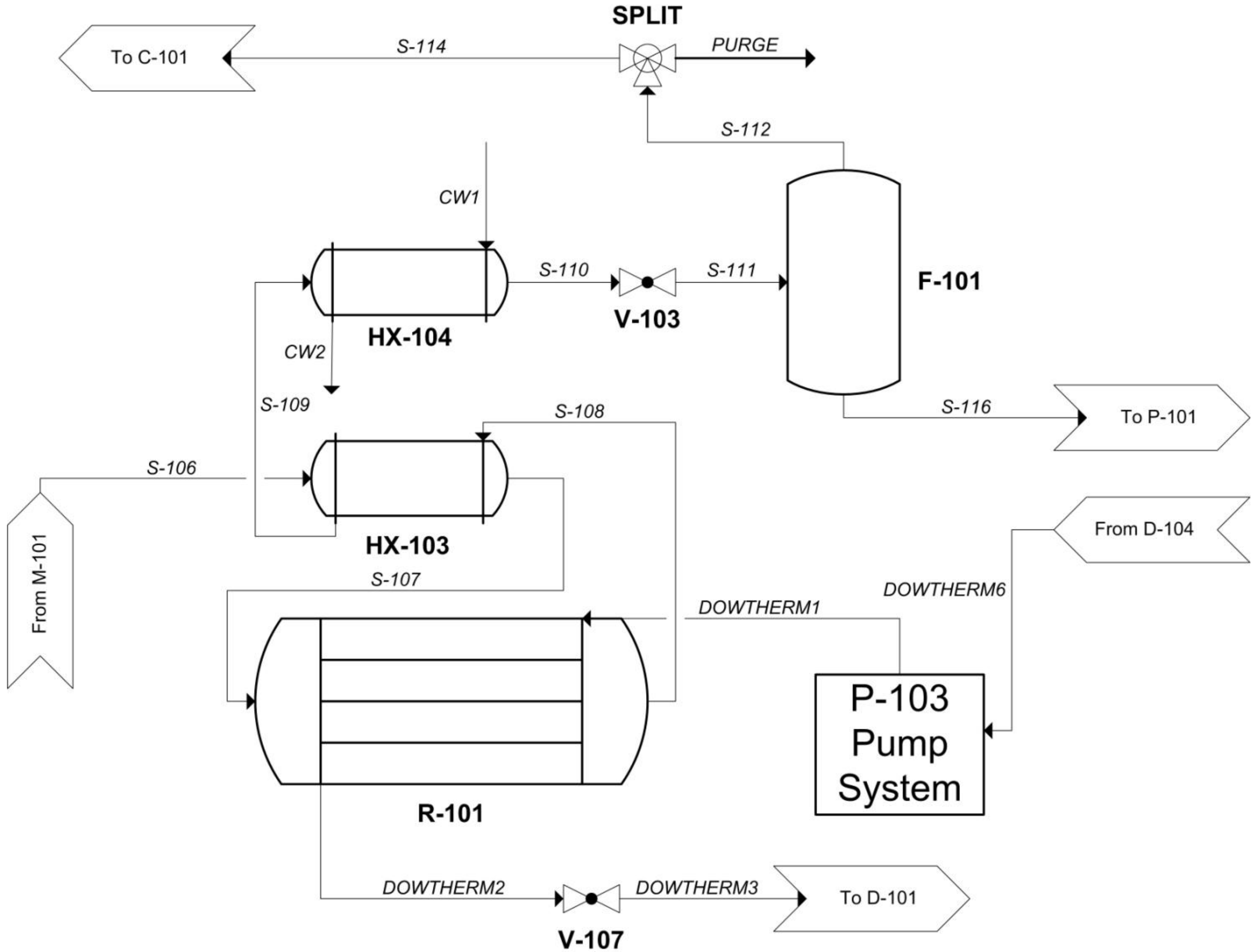

Figure 4.3: Reactor Process Diagram. This shows the flowsheet for the reactor section of the process, which includes the Dowtherm cooling loop and flash drum.

Table 1.3: Reactor Stream Summary. This table provides temperature, pressure, vapor fraction, and component flow rates for all streams in the reactor section of the process flowsheet.

Stream	S-114	PURGE	S-106	S-109	S-110	S-111	S-112	S-116	S-107	S-108
Temperature (°F)	85	85	228	280	85	82	85	85	740	780
Pressure (psia)	25	25	54	40	35	30	25	25	49	45
Vapor Fraction	1	1	1	1	0.92	0.92	1	0	1	1
Total Flow (lb/hr)	55449	1714	62023	62023	62023	62023	57163	4859	62023	62023
Component Flows										
Propane	15382	4757	18025	16223	16223	16223	15857	3651	18025	16223
Oxygen	2427	75	2921	2505	2505	2505	2502	3	2921	2505
Propylene	1914	592	1945	2011	2011	2011	1973	380	1945	2011
Acrylic Acid	1791	55	1901	2854	2854	2854	1846	2670	1901	2854
Water	5713	177	7547	2230	2230	2230	5890	1641	7547	2230
Nitrogen	31341	9693	32324	32324	32324	32324	32311	130	32324	32324
Acetic Acid	379	12	537	1393	1393	1393	390	1003	537	1393
Carbon Dioxide	5779	1788	5809	5989	5989	5989	5958	308	5809	5989
Dowtherm	0	0	0	0	0	0	0	0	0	0

Stream	DOWTHERM-1	DOWTHERM-6	DOWTHERM-2	DOWTHERM-3
Temperature (°F)	198	198	738	458
Pressure (psia)	40	15	35	30
Vapor Fraction	0	0	0	0
Total Flow (lb/hr)	385000	385000	385000	385000
Component Flows				
Dowtherm	385000	385000	385000	385000

4.4 Separation Section

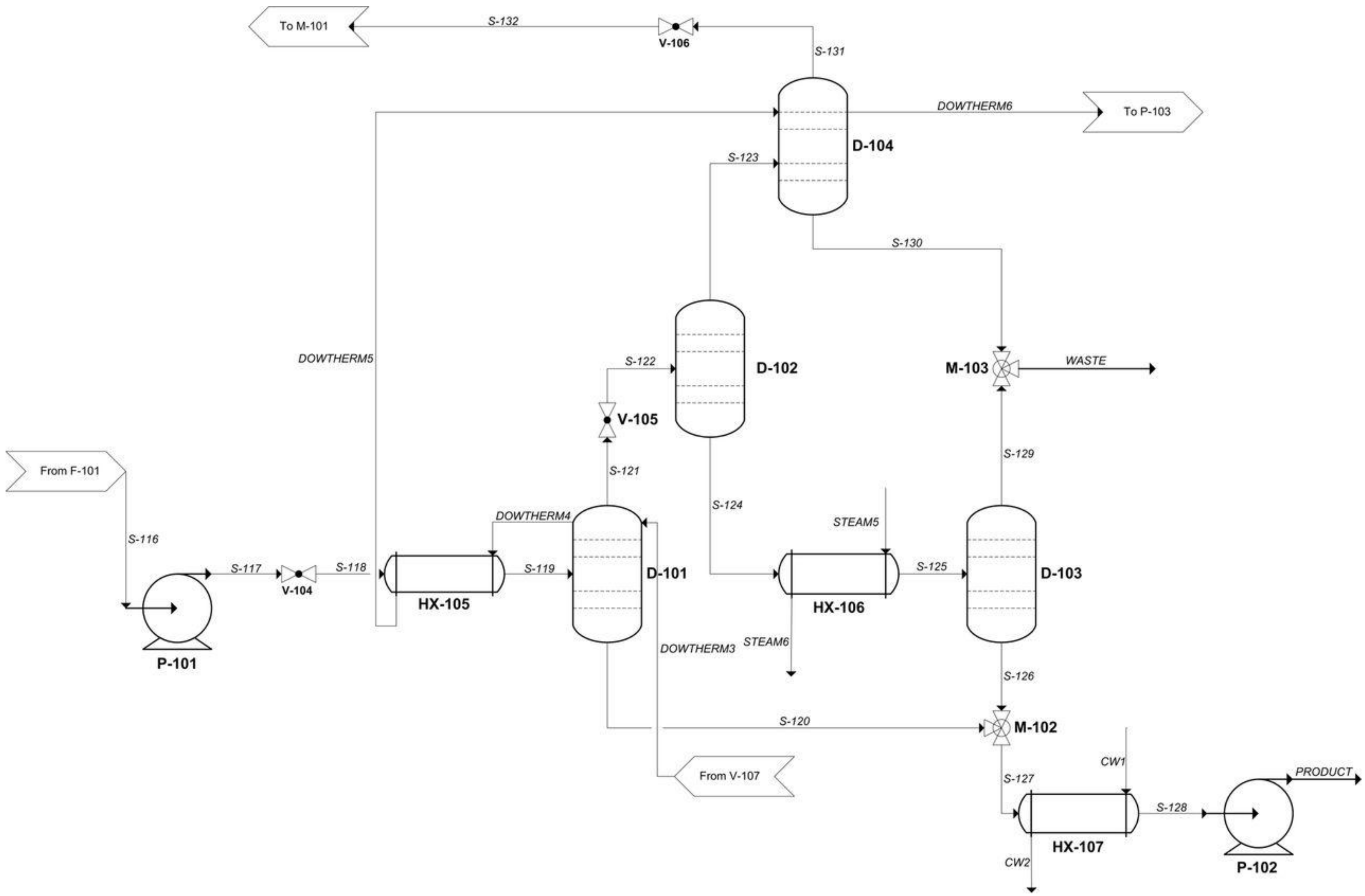

Figure 4.4: Separation Process Diagram. This shows the flowsheet of the separation section of the process, which includes the four distillation towers and the Dowtherm heating loop.

Table 4.4: Separation Process Stream Summary. This table provides temperature, pressure, vapor fraction, and component flow rates for all streams in the separation section of the process flowsheet.

Stream	**S-116**	**S-117**	**S-118**	**S-119**	**S-120**	**S-121**	**S-122**	**S-123**	**S-124**
Temperature (°F)	85	86	86	400	418	318	317	295	307
Pressure (psia)	25	150	130	125	98	95	90	70	73
Vapor Fraction	0	0	0	1	0	1	1	1	0
Total Flow (lb/hr)	48596	48596	48596	48596	23846	24750	24750	19472	5278
Component Flows									
Propane	3651	3651	3651	3651	0	3651	3651	3651	0
Oxygen	3	3	3	3	0	3	3	3	0
Propylene	380	380	380	380	0	380	380	380	0
Acrylic Acid	26702	26702	26702	26702	23844	2858	2858	1024	1834
Water	16419	16419	16419	16419	0	16419	16419	13036	3383
Nitrogen	130	130	130	130	0	130	130	130	0
Acetic Acid	1003	1003	1003	1003	1	1001	1001	941	60
Carbon Dioxide	308	308	308	308	0	308	308	308	0
Dowtherm	0	0	0	0	0	0	0	0	0

Stream	**S-125**	**S-126**	**S-127**	**S-128**	**S-129**	**S-130**	**S-131**	**S-132**	**WASTE**
Temperature (°F)	374	371	415	100	298	287	265	264	236
Pressure (psia)	68	68	68	63	65	67	65	60	25
Vapor Fraction	1	0	0	1	1	0	1	1	0.3
Total Flow (lb/hr)	5278	1469	25314	25314	3809	13819	5653	5653	17628
Component Flows									
Propane	0	0	0	0	0	834	2817	2817	834
Oxygen	0	0	0	0	0	0	3	3	0
Propylene	0	0	0	0	0	75	305	305	75
Acrylic Acid	1834	1443	25286	25286	392	913	110	110	1305
Water	3383	25	25	25	3358	11202	1834	1834	14560
Nitrogen	0	0	0	0	0	0	130	130	0
Acetic Acid	60	1	3	3	59	783	158	158	842
Carbon Dioxide	0	0	0	0	0	12	296	296	12
Dowtherm	0	0	0	0	0	0	0	0	0

Stream	**DOWTHERM-3**	**DOWTHERM-4**	**DOWTHERM-5**	**DOWTHERM-6**
Temperature (°F)	458	299	203	198
Pressure (psia)	30	25	20	15
Vapor Fraction	0	0	0	0
Total Flow (lb/hr)	385000	385000	385000	385000
Component Flows (lb/hr)				
Dowtherm	385000	385000	385000	385000

Section 5

Process Description

5.1 Reactor Section

The conversion of propane to acrylic acid through propylene requires contacting the paraffin with a mixed metal oxide catalyst at approximately 750°F. Since the reaction is highly exothermic, a fixed bed reactor configured as a shell and tube heat exchanger was used, with Dowtherm A as the coolant. The flowsheet for the reactor section can be seen in Figure 4.3, page 22.

Reactor

The reactor dimensions were chosen to ensure both adequate volume for chemical conversion and adequate surface area for sufficient cooling. Based on patent data, the fixed bed reactor, R-101, needs 160 lb catalyst for a space velocity of 1662 hr^{-1}. Given the required feed flow rate, the minimum reactor volume to ensure this space velocity is 670 ft^3. The actual reactor volume is 700 ft^3, allowing 30 ft^3 to be used to adjust the reaction extent with inert ceramic beads or additional catalyst. These beads will also help ensure operating temperature conditions are more consistent with researched conditions. The minimum required surface area for cooling is 11,800 ft^2, which is safely under designed reactor surface area of 16,755 ft^2. The required cooling surface area is based on an estimated overall heat transfer coefficient of 100 Btu/ft^2-hr and a log-mean temperature difference of 100°F.

Table 5.1: Reactor Specifications

Reactor Specifications	
Number of Tubes	4000
Tube Length (ft)	8
Inner - Tube Diameter (in)	2
Pressure Drop (psi)	6

Based on the number of tubes, tube length, and tube diameter, the resulting pressure drop across the reactor is calculated to be approximately 6 psi using the Ergun equation. The feed to the fixed bed reactor is pre-heated to 740°F using the reactor effluent, at 780°F, as a heat source. In order to control the reaction, feed conditions are set such that oxygen is the limiting reactant.

Dowtherm Cooling

Due to the high operating temperature of the reactor and the highly exothermic nature of the reaction, it is necessary to cool the reactor with a Dowtherm stream. The Dowtherm enters the reactor at approximately 198°F and exits at about 738°F. After exiting the reactor, the Dowtherm is used as a heat source for the reboiler of tower D-101, heat exchanger HX-105, and the reboiler of tower D-104, where it provides 54,100,000 Btu/hr, 28,000,000 Btu/hr, and 13,800,000 Btu/hr of heat, respectively. This brings the Dowtherm temperature back down to 203°F. Additional heat losses through the piping system brings the temperature of the Dowtherm back down to the 198°F. In order for the Dowtherm to flow through the piping and three heat exchangers, it is pressurized to 45 psia using a set of 20 pumps setup in parallel.

5.2 Separation

The separation scheme for this process involves one flash drum and four distillation towers. The flowsheet for the separation section of the process can be seen in Figure 4.4, page 24. The main challenge was to isolate acrylic acid from water and acetic acid since these three chemical species form three separate azeotropes: water/acrylic acid, water/acetic acid, and acrylic acid/acetic acid form an azeotrope. Rather than trying to break the azeotropes, this separation scheme avoided them by performing the separation in a specific order. The first tower (D-101) recovers a pure stream of acrylic acid. The second tower (D-102) removes most of the water and acetic acid from the remaining acrylic acid, which is recovered in the third tower (D-103). The fourth tower removes the remaining propane, which is recycled, from the water and acetic acid which exits as wastewater (in addition to the distillate from the third tower).

Flash Drum

The reactor effluent (S-111) was first sent to a flash drum (F-101), where virtually all the propane, oxygen, nitrogen, carbon dioxide, and propylene exits as vapor and the acrylic acid exits as liquid. About 70% of the water and acetic acid exits in the liquid phase and the balance exits in the vapor phase. The vapor from the flash drum is recycled back as reactor feed, while the liquid is fed to the first distillation tower (D-101).

Tower 1

D-101 separates acrylic acid from the reaction byproducts and leftover reactants. About 75% of the acrylic acid produced is recovered in the bottoms (S-120) of this tower. The propane, propylene, carbon dioxide, nitrogen, acetic acid, and water leaves in the distillate (S-121), along with the remaining 25% of the acrylic acid.

Tower 2

D-102 removes propane, propylene, carbon dioxide, and nitrogen from the acrylic acid. It also removes some of the water and acetic acid from the acrylic acid. The distillate from D-101 is the feed to this tower. About 82% of the unrecovered acrylic acid leaves in the bottoms (S-124) and the rest leaves in the distillate (S-123). All the propane, propylene, carbon dioxide, and nitrogen leave this tower in the distillate. About 78% of the water leaves in the distillate along with 87% of the acetic acid, while the balance leaves in the bottoms.

Tower 3

D-103 separates acrylic acid from the remaining water and acetic acid. All the water and acetic acid entering this tower leaves in the distillate (S-129). About 85% of the acrylic acid entering this tower is recovered in the bottoms (S-126) and the balance leaves in the distillate.

Tower 4

D-104 separates the water and acetic acid, which leave as bottoms (S-130), from the propane, propylene, carbon dioxide, and nitrogen, which are recycled (S-131). About 90% of the acrylic acid that enters this tower leaves as bottoms. All the carbon dioxide and nitrogen leave this tower in the distillate (S-131). About 80% of the propane and propylene leave in the distillate, while the remaining 20% leave in the bottoms as wastewater. About 85% of the water and acetic acid that entered this tower leave in the bottoms and the balance leaves in the distillate.

Recovery of Acrylic Acid

About 28,550 lb acrylic acid exit the reactor (R-101) each hour and enter the flash drum (F-101), which is the first separation unit. The first product stream (S-120) has about 23,800 lb of acrylic acid and the second product stream (S-126) has about 1,450 lb acrylic acid. This gives an overall acrylic acid recovery of about 89%. About 5% exits the process in wastewater (WASTE).

5.3 Other Assumptions

Deriving Propane to Propylene Kinetic Expression

The reaction forming propylene from propane is the first step in forming all of the observed products. It is known that the rate-limiting step is the reaction between propane and an open site on the catalytic surface, as is evidenced by the observed kinetics.[13] It is assumed that all subsequent reactions are rapid, and that the size of the pipe reactor required for the target of 10% conversion of propane can be estimated using the known kinetics of the propane to propylene reaction.

Widi et al. performed a kinetic study of propane over a diluted $Mo_1V_{0.30}Te_{0.23}Nb_{0.125}O_x$ catalyst.[14] By varying the feed composition, they were able to obtain the reaction rate for the formation of propylene as a function of propane and oxygen concentrations. They found that the rate expression was first order in propane and zero order in oxygen, and is be approximated by

$$rate \approx k[C_3H_8]^1[O_2]^0 \tag{9}$$

At 673°K, the rate of propylene formation was found to be 0.8 mol/h-g catalyst at a propane concentration of 0.3 mol/L. Assuming a catalyst loading of 1 g, this corresponds to a *k* value of 0.267 hr^{-1}, or 7.41 x 10^{-5} s^{-1}. Using the Arrhenius equation and solving for the pre-exponential factor (*A*):

$$A = k \cdot exp^{\frac{E_a}{RT}} \tag{10}$$

The pre-exponential factor was found to be 4.62 per gram of catalyst, and Widi et al. computed an activation energy value for the formation of propylene of 62.7 kJ/mol, allowing the estimation of a complete kinetic expression for the propane to propylene reaction.

$$k = 4.62 \cdot exp^{\frac{-62,700}{RT}} \tag{11}$$

Kinetics Simplification

Currently, no experimental rate law has been determined for the production of acrylic acid from propylene over a mixed metal oxide catalyst. Thus, selectivities and conversions from patents and journal articles were used to scale up the proposed design process as seen in Figure 5.1, page 33, from (Widi et al., 2009). It is observed that selectivity of propylene decreases as propane conversion increases and that the selectivity to acrylic acid increases as propane

[13] Widi, R. K. (2012). Kinetic Investigation of Carbon Dioxid, Acetic Acid, Acrylic Acid Formation on Diluted and Leached MoVTeNb Catalyst. Indonesian Journal of Chemistry, 12(2), 131-134.
[14] Widi, R. K., Hamid, S. B. A., & Schlogl, R. (2009). Kinetic investigation of propane oxidation on diluted Mo1-V0.3-Te0.23-Nb0.125-Ox mixed-oxide catalysts. Reaction Kinetics and Catalysis Letters, 98, 273-286.

conversion is increased. Selectivities of acetic acid and carbon dioxide remain relatively constant.[15]

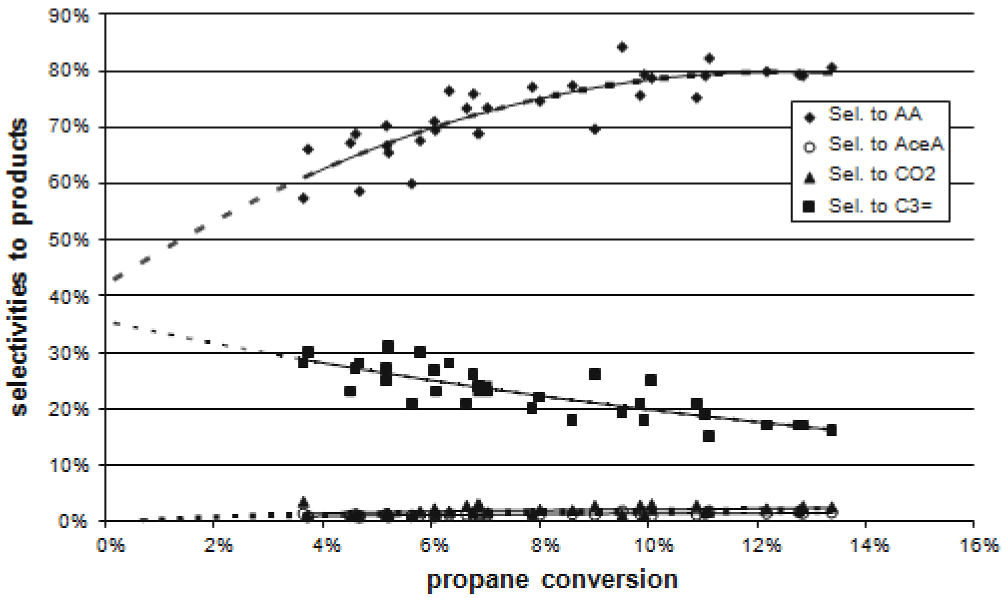

Figure 5.1: Product Selectivity Profiled for Propane Oxidation Over Diluted MoVTeNb Mixed Oxide Catalyst

Aspen Plus Simulation

The APSEN Plus simulations use the NRTL-RK property method. Due to the complex interactions between acrylic acid, acetic acid, and water, three separate azeotropes form. In order to accurately model these azeotropes, 5 additional binary interaction databanks needed to be loaded. VLE-RK, VLE-HOC, VLE-IG, LLE-Aspen, and VLE-LIT were loaded to improve the complex interaction modeling.

Catalyst Assumptions

This process uses a mixed metal oxide catalyst that is not commercially produced at the time of this report. While conversions and selectivities, which were used in modeling the reactor for scale-up, are known, there is no market information on cost. In order to estimate a cost, it was recommended to price the catalyst as bismuth molybdate. This estimation would give a reasonable frame of reference and allow for the catalyst cost to be included in the economic

[15] Widi, R. K. (2012). Kinetic Investigation of Carbon Dioxid, Acetic Acid, Acrylic Acid Formation on Diluted and Leached MoVTeNb Catalyst. Indonesian Journal of Chemistry, 12(2), 131-134.

analysis of this process. It is also assumed that the catalyst needs to be replaced every two years. Additionally, it is estimated that the spent catalyst can be sold back to the supplier as raw material for 15% of the purchase price.

Propane Supply

Based on the proposed site location, it is assumed that propane will be supplied via pipeline for $0.213 per pound. It is further assumed that the propane is arriving in liquid form at standard ambient temperature (75°F), which sets its pressure at 150 psia.

Pure Oxygen Supply

Based on the proposed site location, it is also assumed that pure oxygen can be accessed via pipeline at 500 psig and standard ambient temperature (75°F) for $0.03 per pound.

Wastewater Treatment

It is assumed that a wastewater treatment system already exists on site (or nearby). Therefore, the economic analysis of this design does not include the installation of a wastewater treatment plant. Instead, the analysis includes the cost associated with wastewater treatment based on the hydro-loading and organic compositions of the wastewater streams.

Purge

It is assumed that a furnace for burning the purge gas stream already exists on site (or nearby). Therefore, this design does not include the installation cost of a furnace in the economic analysis. The heating value for this stream was calculated, as well as its dollar value should it be sold to another local facility. The heating value can be used as a credit to offset the utility demand of the plant.

Utility Usage

It is assumed that utilities are readily available for purchase from public or private entities in the Gulf Coast Region where the plant would be located. Utility prices are estimated using Table 23.1 of Product and Process Design, by Seider, Seader, and Lewin. The figures are adjusted to 2013 prices using a CE value of 575.

Section 6

Equipment List & Unit Descriptions

Table 6.1: Equipment List

Equipment Description	Type	Purchase Cost	Bare Module Cost
C-101	Process Machinery	$4,329,750	$13,898,498
C-102	Process Machinery	$1,226,736	$3,937,824
HX-101	Process Machinery	$19,864	$62,968
HX-102	Process Machinery	$21,641	$68,602
HX-103-A	Process Machinery	$668,045	$2,117,704
HX-104	Process Machinery	$239,932	$760,584
HX-105	Process Machinery	$113,536	$359,910
HX-106	Process Machinery	$21,432	$67,939
HX-107	Process Machinery	$27,077	$85,835
F-101	Process Machinery	$204,355	$655,980
P-101	Process Machinery	$22,373	$73,830
P-101- backup	Spares	$22,373	$73,830
P-102	Process Machinery	$5,645	$18,630
P-102-backup	Spares	$5,645	$18,630
P-103 x20	Process Machinery	$1,070,080	$3,434,957
P-103-backup x20	Spares	$1,070,080	$3,434,957
D-101-C	Process Machinery	$109,459	$351,364
D-101-RA	Process Machinery	$37,636	$120,813
D-101-REB	Process Machinery	$1,312,882	$4,214,351
D-101-P	Process Machinery	$9,305	$30,705
D-101-P-backup	Spares	$9,305	$30,705
D-101	Process Machinery	$734,641	$3,048,760
D-102-C	Process Machinery	$112,282	$360,425
D-102-RA	Process Machinery	$28,645	$91,952
D-102-REB	Process Machinery	$766,632	$2,460,888
D-102-P	Process Machinery	$8,573	$28,290
D-102-P-backup	Spares	$8,573	$28,290
D-102	Process Machinery	$354,514	$1,471,232
D-103-C	Process Machinery	$29,064	$93,294
D-103-RA	Process Machinery	$17,459	$56,044
D-103-REB	Process Machinery	$74,855	$240,283
D-103-P	Process Machinery	$6,377	$21,045
D-103-P-backup	Spares	$6,377	$21,045
D-103	Process Machinery	$282,273	$1,171,432
D-104-C	Process Machinery	$36,695	$117,792
D-104-RA	Process Machinery	$19,864	$63,762
D-104-REB	Process Machinery	$21,327	$68,461
D-104-P	Process Machinery	$6,586	$21,735
D-104-P-backup	Spares	$6,586	$21,735
D-104	Process Machinery	$98,900	$410,435
T-101	Process Machinery	$176,055	$565,135
Reactor	Process Machinery	$281,390	$903,262
Storage Tank- Propane	Storage	$168,131	$512,797
Storage Tank- Acrylic Acid	Storage	$291,705	$291,705
Catalyst	Catalysts	$5,576,741	$5,576,741
Dowtherm	Other Equipment	$699,530	$699,530
Total		***$20,360,926***	***$52,191,590***

Of the $52,191,590 total bare module cost, approximately 27% comes from the large compressor. This is due to the large scale of the compressor, which compresses 3,926,000 ft^3/hr of reactant by 24 psi (starting at 85°F).

Costing for most equipment was based on values provided by Aspen IPE. Aspen result reports for the blocks are shown in Appendix B (starting on p. 149). Other process units are discussed in detail in the appropriate section, with associated Aspen results and design calculations referenced. All equipment that comes in contact with product streams (including recycle) are made using stainless steel 304 to prevent reactions between equipment material and organic acids.

6.1 Unit Descriptions

Pumps

Sample calculations for determining pump head and electricity requirements are provided in Appendix C, page 184. All pumps in the process have spares which were included in the calculation of total bare module costs. Each pump was assumed to have a single spare at equivalent purchase and bare module cost.

P-101 - Base Purchase Cost: $22,373

This is a centrifugal pump constructed of stainless steel that sends the liquid product of the flash vessel through the separation process. S-116 flows at a rate of 48,596 lb/hr and a temperature of 86°F. The pump has an efficiency of 0.537, a brake power of 13.8 hp, and a pump head of 301.8 ft. It raises the pressure of the stream from 24.7 psia to 150 psia.

D-101-P - Base Purchase Cost: $9,305

This is a centrifugal pump constructed of stainless steel that sends the liquid reflux of D-101 through the tower. The pump pushes liquid at a rate of 238 gpm and operates at 119.6 psia and 368°F. The pump has a brake power of 20 hp and a pump head of 225 ft.

D-102-P – Base Purchase Cost: $8,573

This is a centrifugal pump constructed of stainless steel that sends the liquid reflux of D-102 through the tower. The pump pushes liquid at a rate of 200 gpm and operates at 90.3 psia and 345°F. The pump has a brake power of 15 hp and a pump head of 225 ft.

D-103-P – Base Purchase Cost: $6,377

This is a centrifugal pump constructed of stainless steel that sends the liquid reflux of D-103 through the tower. The pump pushes liquid at a rate of 29.9 gpm and operates at 75.3 psia and 348°F. The pump has a brake power of 3 hp and a pump head of 225 ft.

D-104-P – Base Purchase Cost: $6,586

This is a centrifugal pump constructed of stainless steel that sends the liquid reflux of D-104 through the tower. The pump pushes liquid at a rate of 60.4 gpm and operates at 75.3 psia and 315°F. The pump has a brake power of 5 hp and a pump head of 225 ft.

P-102 - Base Purchase Cost: $5,645

This is a centrifugal pump constructed of stainless steel that sends the liquid product to the storage tank. S-128 flows at a rate of 25,286 lb/hr and a temperature of 100°F. The pump has an efficiency of 0.437, a brake power of 0.785 hp, and a pump head of 26.8 ft. It raises the pressure of the stream from 63 psia to 75 psia.

P-103 - Base Purchase Cost: $53,504

This is a system of 20 pumps that pressurize the Dowtherm cooling/heating system. Dowtherm flows at a rate of 25,314 lb/hr and a temperature of 198°F through each pump. The pump has an efficiency of 0.83, a brake power of 15,764 hp, and a pump head of 1,037 ft. It raises the pressure of the Dowtherm from 15 psia to 40 psia.

Flash Vessels

Flash Vessel calculations were based on Aspen simulations, which used an NRTL-RK thermodynamic model, summarized in the input summary provided in Appendix B, page 156.

F-101 - Base Purchase Cost: $204,355

This stainless steel flash column separates the products of the reaction from the reactants. S-111 enters at a rate of 620,230 lb/hr. The bottoms product (S-116), containing the product, is sent through the separation section at a rate of 48,596 lb/hr. The vapor (S-112) is sent back to the reactor at a rate of 571,634 lb/hr. The tower operates at 85°F and 25 psia. It has a diameter of 16.5 feet, a height of 12 ft, and a wall thickness of 0.3125 in.

Heat Exchangers

Sample calculations for determining the heat duty, heat transfer coefficient, heat transfer area, and utility requirements for these shell-tube heat exchangers are provided in Appendix C, page 178.

HX-101 - Base Purchase Cost: $19,864

This carbon steel shell and tube heat exchanger heats up stream S-100 using pressurized steam. S-100 enters at a temperature of -106°F and exits as S-102 at a temperature of 230°F. S-100 flows through the tube side of the heat exchanger at a rate of 23,839 lb/hr. Steam moves at a flow rate of 1,998 lb/hr and a temperature of 328°F through the shell side of the exchanger. The overall surface area of the exchanger is 172 ft^2, and the overall heat duty is 1,775,817 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

HX-102 - Base Purchase Cost: $21,641

This carbon steel shell and tube heat exchanger heats up stream S-104 using pressurized steam. S-100 enters at a temperature of 24°F and exits as S-105 at a temperature of 230°F. S-104 flows through the tube side of the heat exchanger at a rate of 23,615 lb/hr. Steam moves at a flow rate of 5,885 lb/hr and a temperature of 328°F through the shell side of the exchanger. The overall surface area of the exchanger is 207 ft^2, and the overall heat duty is 5,230,767 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

HX-103 - Base Purchase Cost: $668,045

This stainless steel shell and tube heat exchanger heats up the reactor feed using the reactor effluent. S-108 (feed) enters at a temperature of 230°F and exits as S-107 at a temperature of 740°F, at a rate of 620,230 lb/hr through the shell side. S-108 (effluent) enters at a temperature of 780°F and exits as S-109 at a temperature of 280°F, at a rate of 620,230 lb/hr through the tube side. The overall surface area of the exchanger is 12,595 ft^2, and the overall heat duty is

118,783,845 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

R-101 - Base Purchase Cost: $281,389

This carbon steel (shell)/stainless steel (tube) exchanger acts as the reactor system. The reactor is designed to have 4,000 eight-foot tubes that are filled with catalyst and that have a 2 in inner diameter (2.375 in outer diameter) and a pitch of 3 in. The space velocity of the reactor/flow system is 1662 hr^{-1}, with a residence time of 2.17 sec. The bed porosity is estimated to be 0.4. The catalyst contains 30 ft^3 inert (such as ceramic beads) for better heat transfer through the system. The U was assumed to be 100 BTU/hr-ft^2-°F. S-107 enters at a temperature of 740°F at a rate of 620,230 lb/hr, and heats to 780°F. Dowtherm A is used to cool the reactor. It enters the reactor at 198°F at a rate of 385,000 lb/hr, and exits at 738°F. The overall surface area of the reactor is designed to be 16,755 ft^2. The overall heat duty, as calculated from heat of reaction and conversion data, is estimated to be 120,000,000 BTU/hr.

HX-104 - Base Purchase Cost: $239,932

This carbon steel (shell)/stainless steel (tube) exchanger cools the product stream before it enters F-101. S-109 enters at a temperature of 280°F and exits as S-110 at a temperature of 85°F, at a rate of 620,230 lb/hr through the tube side. Cooling water enters at a temperature of 75°F and exits as 95°F, at a rate of 3,149,831 lb/hr through the shell side. The overall surface area of the exchanger is 6,368 ft^2, and the overall heat duty is 63,053,511 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

HX-105 - Base Purchase Cost: $113,536

This stainless steel shell and tube heat exchanger heats the product stream before it enters tower D-101. S-118 enters at a temperature of 86°F and exits at a temperature of 400°F, at a flow rate of 48,596 lb/hr. Dowtherm A travels through the shell at a flow rate of 385,000 lb/hr, cooling from 458°F to 299°F. The overall surface area of the exchanger is 1,821 ft^2, and the overall heat duty is 27,876,354 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

D-101-C - Base Purchase Cost: $109,459

This stainless steel (tube)/carbon steel (shell) exchanger acts as the condenser for tower D-101. S-C-1 flows through the exchanger at a rate of 24,750 lb/hr. Cooling water flows at a rate of 2,931,977 lb/hr, heating from 75°F to 95°F. The surface area of the exchanger is 1,925 ft^2, and has a heat duty of 58,692,479 BTU/hr. The diameter of the shell is 27 in. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

D-101-REB - Base Purchase Cost: $1,312,882

This stainless steel (tube)/carbon steel (shell) u-tube kettle acts as the reboiler for tower D-101. S-R-1 flows through the exchanger at a rate of 23,846 lb/hr. DOWTHERM acts as the heat source, and flows at a rate of 385,000 lb/hr, cooling from 738°F to 458°F, and has a heat duty of 54,062,820 BTU/hr. The diameter of the shell is 67 in, there are 7 shells total, and the surface area in each shell is 2,729 ft^2. The tubes have an outer diameter of 1 in, are 13 ft long, and have a pitch of 1.25.

D-102-C - Base Purchase Cost: $112,282

This stainless steel (tube)/carbon steel (shell) exchanger acts as the condenser for tower D-102. S-C-3 flows through the exchanger at a rate of 19,472 lb/hr. Cooling water flows at a rate of 2,763,294 lb/hr, heating from 75°F to 95°F. The surface area of the exchanger is 2,003 ft^2, and has a heat duty of 55,315,822 BTU/hr. The diameter of the shell is 27 in. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

D-102-REB - Base Purchase Cost: $766,632

This stainless steel (tube)/carbon steel (shell) u-tube kettle acts as the reboiler for tower D-102. S-R-3 flows through the exchanger at a rate of 5,278 lb/hr. Pressurized steam at 100 psia and 328°F flows at a rate of 58,243 lb/hr. The exchanger has a heat duty of 51,760,761 BTU/hr. The diameter of the shell is 66 in, there are 5 shells total, and the surface area in each shell is 2,581 ft^2. The tubes have an outer diameter of 1 in, are 13 ft long, and have a pitch of 1.25.

D-103-C - Base Purchase Cost: $29,064

This stainless steel (tube)/carbon steel (shell) exchanger acts as the condenser for tower D-103. S-C-5 flows through the exchanger at a rate of 3,809 lb/hr. Cooling water flows at a rate of 470,853 lb/hr, heating from 75°F to 95°F. The surface area of the exchanger is 341 ft^2, and has a heat duty of 9,425,587 BTU/hr. The diameter of the shell is 12 in. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

D-103-REB - Base Purchase Cost: $74,955

This stainless steel (tube)/carbon steel (shell) u-tube kettle acts as the reboiler for tower D-103. S-R-5 flows through the exchanger at a rate of 1,469 lb/hr. Pressurized steam at 400 psia and 445°F flows at a rate of 11,572 lb/hr. The exchanger has a heat duty of 9,030,477 BTU/hr. The diameter of the shell is 44 in and the surface area of the exchanger is 962 ft^2. The tubes have an outer diameter of 1 in, are 13 ft long, and have a pitch of 1.25.

D-104-C - Base Purchase Cost: $36,695

This stainless steel (tube)/carbon steel (shell) exchanger acts as the condenser for tower D-104. S-C-7 flows through the exchanger at a rate of 5,653 lb/hr. Cooling water flows at a rate of 608,848 lb/hr, heating from 75°F to 95°F. The surface area of the exchanger is 507 ft^2, and has a heat duty of 12,187,883 BTU/hr. The diameter of the shell is 14 in. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

D-104-REB - Base Purchase Cost: $21,327

This stainless steel (tube)/carbon steel (shell) u-tube kettle acts as the reboiler for tower D-104. S-R-7 flows through the exchanger at a rate of 13,819 lb/hr. DOWTHERM acts as the heat source, and flows at a rate of 385,000 lb/hr, cooling from 299°F to 213°F, and has a heat duty of 1,380,582 BTU/hr. The diameter of the shell is 18 in and the surface area of the exchanger is 157 ft^2. The tubes have an outer diameter of 1 in, are 13 ft long, and have a pitch of 1.25.

HX-107 - Base Purchase Cost: $27,077

This carbon steel (shell)/stainless steel (tube) exchanger cools the product stream before it enters storage. S-127 enters at a temperature of 415°F and exits as S-128 at a temperature of 100°F, at a rate of 25,286 lb/hr through the tube side. Cooling water enters at a temperature of 75°F and exits as 95°F, at a rate of 123,738 lb/hr through the shell side. The overall surface area of the exchanger is 314 ft^2, and the overall heat duty is 2,476,950 BTU/hr. The tubes have an outer diameter of 1 in, are 20 ft long, and have a pitch of 1.25.

Distillation Columns

Sample calculations for determining the height, diameter, reflux ratio, shell thickness for the distillation columns are provided in Appendix C on page 168-169. A tray efficiency calculation for the distillation column is provided in Appendix C on page 171.

D-101 - Purchase cost: $734,641

This stainless steel distillation column is used to easily separate a bulk of the acrylic acid product. Stream S-119 enters on stage 6 at a rate of 48,596 lb/hr. The column has a reflux ratio of 3.5, a total of 19 stages, a distillate-to-feed ratio of 0.764, and uses a partial-vapor condenser. It is designed to be 50 ft tall with a diameter of 12 ft and 0.75 in shell thickness. The top tray has a temperature of 320ºF and a pressure of 95 psia. The distillate (S-121) flows through a partial-vapor condenser, D-101-C, and into a reflux accumulator, D-101-RA. The bottom tray has a temperature of 418ºF and a pressure of 98.3 psia. The bottoms go through a reboiler, D-101-REB. S-120 exits the bottom of the column at 23,846 lb/hr and is 99.9% acrylic acid by weight. S-121 exits the top of the reactor and is sent to D-102 at a rate of 24750 lb/hr.

D-102 - Purchase cost: $354,514

This stainless steel distillation column is used to separate a bulk of the impurities from the acrylic acid. S-121 enters on stage 11. The column has a reflux ratio of 4, a total of 19 stages, a distillate-to-feed ratio of 0.8, and uses a partial-vapor condenser. It is designed to be 50 ft tall with a diameter of 7 ft and 0.313 in shell thickness. The top tray has a temperature of 295ºF and a pressure of 70 psia. The distillate (S-123) flows through a partial-vapor condenser, D-102-C, and into a reflux accumulator, D-102-RA. The bottom tray has a temperature of 310ºF and a pressure of 73.4 psia. The bottoms go through a reboiler, D-102-REB. S-124 exits the bottom of the column at 5,278 lb/hr and is sent to D-103 and is 34.8% acrylic acid by weight. S-123 exits the top of the reactor and is sent to D-104 at a rate of 19,472 lb/hr and is 5% acrylic acid by weight.

D-103 - Purchase cost: $282,272

This stainless steel distillation column is used to purify the remaining acrylic acid. S-125 enters on stage 11. The column has a reflux ratio of 3, a total of 20 stages, a distillate-to-feed ratio of 0.9, and uses a partial-vapor condenser. It is designed to be 52 ft tall with a diameter of 5.5 ft and 0.25 in shell thickness. The top tray has a temperature of 298ºF and a pressure of 65 psia. The distillate (S-129) flows through a partial-vapor condenser, D-103-C, and into a reflux accumulator, D-103-RA. The bottom tray has a temperature of 389ºF and a pressure of 68.4 psia. The bottoms go through a reboiler, D-103-REB. S-126 exits the bottom of the column at 1,469 lb/hr and is 98.2% acrylic acid by weight. S-129 exits the top of the reactor at a rate of 3,809 lb/hr and is a waste stream sent to a treatment plant (is 88.2% water by weight, rest is organic material).

D-104 - Purchase cost: $98,900

This stainless steel distillation column is used to separate a bulk of the water from the reactants. S-123 enters on stage 2. The column has a reflux ratio of 4, a total of 3 stages, a distillate-to-feed ratio of 0.22, and uses a partial-vapor condenser. It is designed to be 18 ft tall with a diameter of 3.5 ft, and 0.25 in shell thickness. The top tray has a temperature of 264ºF and a pressure of 65 psia. The distillate (S-131) flows through a partial-vapor condenser, D-104-C, and into a reflux accumulator, D-104-RA. The bottom tray has a temperature of 286ºF and a pressure of 67.1 psia. The bottoms go through a reboiler, D-104-REB. S-130 exits the bottom of the column at 13,819 lb/hr and is sent to a waste stream treatment plant (is 81.1% water by weight, rest is organic material). S-131 exits the top of the reactor at a rate of 5,653 lb/hr and is sent back through the reactor.

Reflux Accumulators

Discussion of the mean residence time to determine the volume of the reflux accumulators is provided in Appendix C on page 176.

D-101-RA - Base Purchase Cost: $37,636

The reflux accumulator is a horizontal vessel, with a diameter of 4.5 ft, a length of 13.5 ft, a shell thickness of 0.25 in, and a volume of 191 ft^3. This is based on a residence time of 5 min.

D-102-RA - Base Purchase Cost: $28,645

The reflux accumulator is a horizontal vessel, with a diameter of 4 ft, a length of 12.5 ft, a shell thickness of 0.1875 in, and a volume of 157 ft^3. This is based on a residence time of 5 min.

D-103-RA - Base Purchase Cost: $17,000

The reflux accumulator is a horizontal vessel, with a diameter of 3 ft, a length of 3.5 ft, a shell thickness of 0.1875 in, and a volume of 33 ft^3. This is based on a residence time of 5 min.

D-104-RA - Base Purchase Cost: $19,863

The reflux accumulator is a horizontal vessel, with a diameter of 3 ft, a length of 6.5 ft, a shell thickness of 0.1875 in, and a volume of 61.3 ft^3. This is based on a residence time of 5 min.

Storage Tanks

Sample calculations for determining the volume of the storage tanks are provided in Appendix C, page 185.

STOR-PROP - Base Purchase Cost: $168,131

This carbon steel storage tank holds compressed (150 psia) propane from pipeline (in case of interruption of service). It has a volume of 6,120 gallons. It can store up to eight hour's worth propane. The contents are decompressed, heated, and fed into the reactor at a rate of 23,616 lb/hr.

STOR-PROD - Base Purchase Cost: $291,705

This stainless steel storage tank holds 7 day's worth acrylic acid before shipping. It has a volume of 700,000 gallons. It holds acrylic acid at 15 psia and 75°F.

Compressors & Turbines

Sample calculations for determining the utility and space requirements are provided in Appendix C, page 183.

T-101 - Base Purchase Cost: $176,055

This is a carbon steel turbine used to decompress oxygen from 500 psia to 54 psia. The isentropic efficiency is assumed to be 0.72. Energy from the turbine is put into the grid as energy credits. The flow rate through the turbine is 23,839 lb/hr. The energy created by the turbine is 345 hp.

C-101 - Base Purchase Cost: $4,329,750

This is a stainless steel compressor used to compress S-114 (F-101 vapor) to 59 psia, in order to push the flow back through the reactor loop system. The isentropic efficiency is assumed to be 0.72. The flow rate through the compressor is 554,485 lb/hr. The brake power required for the compressor is 9,294 hp.

C-102 - Base Purchase Cost: $1,226,736

This is a carbon steel compressor used to compress ambient air to 54 psia. The isentropic efficiency is assumed to be 0.72. The flow rate through the compressor is 12,637 lb/hr. The brake power required by the compressor is 400 hp.

6.2 Unit Equipment Sheets

Compressor

Compressor			
Identification	Item: Item No: No. Req'd:	Single-Stage C-101 1	
Function **Operation**	Compresses recycle stream Continuous		
Materials Handled:	**Stream In:** S-114	**Stream Out:** S-115	
Flow Rate (lb/hr)	554,485	554,485	
Temperature (°F)	85	225	
Pressure (psia)	25	59	
Design Data:	Number of Stages		1
	Isentropic Efficiency		0.72
	Total work (hp)		9,294
	Material of Construction		Carbon Steel
Purchase Cost:	$ 4,329,750		
Bare Module Cost	$ 13,898,498		
Utilities (USD/yr):	$ 3,787,380		

Compressor		
Identification	Item: Item No: No. Req'd:	Single-Stage C-102 1
Function **Operation** **Type**	Compresses inlet air Continuous N/A	
Materials Handled:	**Stream In:** AIR	**Stream Out:** S-103
Flow Rate (lb/hr)	12,636	12,636
Temperature (°F)	75	406
Pressure (psia)	14.5	54
Design Data:	Number of Stages Isentropic Efficiency Total work (hp) Material of Construction	1 0.72 400 Carbon Steel
Purchase Cost:	$ 1,226,736	
Bare Module Cost:	$ 3,937,823	
Utilities (USD/yr):	$ 22,342	

Distillation Column

Distillation Column			
Identification	Item:	Distillation Column	
	Item No:	D-101	
	No. Req'd:	1	
Function	Acrylic Acid purificatoin		
Operation	Continuous		
Type	N/A		
Materials Handled:	**Stream In:**	**Streams Out:**	
	(Feed)	(Distillate)	(Bottoms)
	S-119	S-121	S-120
Flow Rate (lb/hr)	48,596	24,750	23,846
Temperature (°F)	48,596	318	418
Pressure (psia)	125	95	98
Composition (mass frac)			
Propane	0.075	0.148	0.000
Propylene	0.008	0.015	0.000
Oxygen	0.000	0.000	0.000
Water	0.338	0.663	0.000
Carbon Dioxide	0.006	0.013	0.000
Nitrogen	0.003	0.005	0.000
Acetic Acid	0.021	0.041	0.000
Acrylic Acid	0.550	0.116	1.000
Design Data:	Actual Stages:		19
	Diameter (ft):		12
	Height (ft):		50
	Shell Thickness (in):		0.75
	Distillate-to-feed ratio (mole):		0.76
	Reflux Ratio		3.5
	Tray Type:		Sieve
	Materials of Construction:		Stainless Steel
Purchase Cost	$ 734,641		
Bare Module Cost	$ 3,048,760		

Distillation Column			
Identification	Item:	Distillation Column	
	Item No:	D-102	
	No. Req'd:	1	
Function	Acrylic Acid purificatoin		
Operation	Continuous		
Type	N/A		
Materials Handled:	**Stream In:**	**Streams Out:**	
	(Feed)	(Distillate)	(Bottoms)
	S-121	S-123	S-124
Flow Rate (lb/hr)	24,750	19,472	5,278
Temperature (°F)	318	295	307
Pressure (psia)	95	70	73
Composition (mass frac)			
Propane	0.148	0.188	0.000
Propylene	0.015	0.020	0.000
Oxygen	0.000	0.000	0.000
Water	0.663	0.670	0.641
Carbon Dioxide	0.013	0.016	0.000
Nitrogen	0.005	0.007	0.000
Acetic Acid	0.041	0.048	0.011
Acrylic Acid	0.116	0.053	0.348
Design Data:	Actual Stages:		19
	Diameter (ft):		7
	Height (ft):		52
	Shell Thickness (in):		0.31
	Distillate-to-feed ratio (mole)		0.8
	Reflux Ratio:		4
	Tray Type:		Sieve
	Materials of Construction:		Stainless Steel
Purchase Cost	$ 354,514		
Bare Module Cost	$ 1,471,232		

Distillation Column			
Identification	Item:	Distillation Column	
	Item No:	D-103	
	No. Req'd:	1	
Function	Acrylic Acid purificatoin		
Operation	Continuous		
Type	N/A		
Materials Handled:	**Stream In:**	**Streams Out:**	
	(Feed)	(Distillate)	(Bottoms)
	S-125	S-129	S-126
Flow Rate (lb/hr)	5,278	3,809	1,469
Temperature (°F)	374	298	371
Pressure (psia)	68	65	68
Composition (mass frac)			
Propane	0.000	0.000	0.000
Propylene	0.000	0.000	0.000
Oxygen	0.000	0.000	0.000
Water	0.641	0.882	0.017
Carbon Dioxide	0.000	0.000	0.000
Nitrogen	0.000	0.000	0.000
Acetic Acid	0.011	0.016	0.000
Acrylic Acid	0.348	0.103	0.982
Design Data:	Actual Stages:		20
	Diameter (ft):		5.5
	Height (ft):		52
	Shell Thickness (in):		0.25
	Distillate-to-feed ratio (mole)		0.9
	Reflux Ratio:		3
	Tray Type:		Sieve
	Materials of Construction:		Stainless Steel
Purchase Cost	$ 282,272		
Bare Module Cost:	$ 1,171,429		

Distillation Column			
Identification	Item:	Distillation Column	
	Item No:	D-104	
	No. Req'd:	1	
Function	Purify recycle		
Operation	Continuous		
Type	N/A		
Materials Handled:	**Stream In:**	**Streams Out:**	
	(Feed)	(Distillate)	(Bottoms)
	S-123	S-131	S-130
Flow Rate (lb/hr)	19,472	5,653	13,819
Temperature (°F)	295	265	287
Pressure (psia)	70	65	67
Composition (mass frac)			
Propane	0.187	0.498	0.060
Propylene	0.020	0.054	0.000
Oxygen	0.000	0.000	0.000
Water	0.670	0.325	0.811
Carbon Dioxide	0.016	0.052	0.000
Nitrogen	0.007	0.023	0.000
Acetic Acid	0.048	0.028	0.057
Acrylic Acid	0.053	0.020	0.066
Design Data:	Stages:		3
	Diameter (ft):		3.5
	Height (ft):		18
	Shell Thickness (in):		0.25
	Distillate-to-feed ratio (mole)		0.22
	Reflux Ratio		4
	Tray Type:		Sieve
	Materials of Construction:		Carbon steel
Purchase Cost:	$ 98,900		
Bare Module Cost:	$ 410,435		

Flash Vessel

Identification	Item:	Flash Drum	
	Item No:	F-101	
	No. Req'd:	1	
Function	Remove high volatility compounds to be recycled		
Operation	Continuous		
Type	2-Phase Flash Drum		
Materials Handled:	**Stream In:**	**Streams Out:**	
	(Feed)	(Vapor)	(Liquid)
	S-111	S-112	S-116
Flow Rate (lb/hr)	620,230	571,634	48,596
Temperature (°F)	82	85	85
Pressure (psia)	30	25	25
Composition (mass frac)			
Propane	0.262	0.277	0.075
Propylene	0.032	0.035	0.008
Oxygen	0.004	0.004	0.000
Water	0.036	0.010	0.338
Carbon Dioxide	0.097	0.104	0.006
Nitrogen	0.521	0.565	0.003
Acetic Acid	0.002	0.001	0.021
Acrylic Acid	0.046	0.003	0.550
Design Data:	Operating Temperature (°F)	85	
	Operating Pressure (psia)	25	
	Diameter (ft)	17	
	Height (ft)	12	
	Volume (ft^3)	2,566	
	Weight (lb)	30,100	
	Heat duty (Btu/hr)	2,383,149	
	Construction Material	Stainless Steel	
Purchase Cost:	$ 204,355		
Bare Module Cost:	**$ 655,980**		

Heat Exchanger

Heat Exchanger		
Identification	Item:	Heater
	Item No:	HX-101
	No. Req'd:	1
Function	Pre-heats decompressed oxygen feed	
Operation	Continuous	
Type	Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-101	STEAM1
Stream Out	S-102	STEAM2
Flow Rate (lb/hr)	23,839	1,998
Inlet Temperature (°F)	-106	328
Outlet Temperature (°F)	230	328
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	172
	Tube pitch (in)	1.25
	ΔTlm (°F)	226
	Heat Duty (Btu/hr)	1,775,817
	Total weight (lb)	2,000
	Construction Materials (Shell/Tube)	Carbon Steel/Carbon Steel
Purchase Cost	$ 19,864	
Bare Module Cost	$ 62,968	
Utilities (USD/yr):	$ 134,678	

Heat Exchanger		
Identification	Item: Item No: No. Req'd:	Heater HX-102 1
Function **Operation** **Type**	Pre-heats decompressed propane feed Continuous Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-104	STEAM3
Stream Out	S-105	STEAM4
Flow Rate (lb/hr)	23,616	5,886
Inlet Temperature (°F)	24	328
Outlet Temperature (°F)	230	328
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	206
	Tube pitch (in)	1.25
	ΔTlm (°F)	182
	Heat Duty (Btu/hr)	5,230,767
	Total weight (lb)	2,200
	Construction Materials (Shell/Tube)	Carbon Steel/Carbon Steel
Purchase Cost	$ 21,641	
Bare Module Cost	$ 68,602	
Utilities (USD/yr):	$ 396,703	

Heat Exchanger		
Identification	Item:	Heat Exchanger
	Item No:	HX-103
	No. Req'd:	1
Function	Uses heat from reactor effluent to pre-heat reactor feed	
Operation	Continuous	
Type	Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-108	S-106
Stream Out	S-109	S-107
Flow Rate (lb/hr)	620,230	620,230
Inlet Temperature (°F)	780	228
Outlet Temperature (°F)	280	740
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	12,595
	Tube pitch (in)	1
	ΔTlm (°F)	46
	Heat Duty (Btu/hr)	118,783,845
	Total weight (lb)	79,800
	Construction Materials (Shell/Tube)	Stainless Steel/Stainless Steel
Purchase Cost	$ 668,045	
Bare Module Cost	$ 2,117,704	
Utilities (USD/yr):	N/A	

Heat Exchanger		
Identification	Item:	Heater
	Item No:	HX-104
	No. Req'd:	1
Function	Cools reactor effluent to enter flash drum F-101	
Operation	Continuous	
Type	Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-109	CW1
Stream Out	S-110	CW2
Flow Rate (lb/hr)	620,230	3,149,831
Inlet Temperature (°F)	280	75
Outlet Temperature (°F)	85	95
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	6,368
	Tube pitch (in)	1
	ΔTlm (°F)	60
	Heat Duty (Btu/hr)	-63,053,511
	Total weight (lb)	39,900
	Construction Materials (Shell/Tube)	Carbon Steel/Stainless steel
Purchase Cost	$ 239,932	
Bare Module Cost	$ 760,584	
Utilities (USD/yr):	$ 375,711.00	

Heat Exchanger		
Identification	Item:	Heater
	Item No:	HX-105
	No. Req'd:	1
Function	Pre-heating for D-101	
Operation	Continuous	
Type	Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-118	DOWTHERM-4
Stream Out	S-119	DOWTHERM-5
Flow Rate (lb/hr)	48,596	385,000
Inlet Temperature (°F)	86	458
Outlet Temperature (°F)	400	299
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	1,821
	Tube pitch (in)	1.25
	ΔTlm (°F)	135
	Heat Duty (Btu/hr)	27,876,354
	Total weight (lb)	14,500
	Construction Materials (Shell/Tube)	Stainless Steel/Stainless Steel
Purchase Cost	$ 113,536	
Bare Module Cost	$ 359,910	
Utilities (USD/yr):	DOWTHERM	

Heat Exchanger		
Identification	Item:	Heater
	Item No:	HX-106
	No. Req'd:	1
Function	Pre-heating for D-103	
Operation	Continuous	
Type	Fixed Head Shell and Tube	
	Tube Side	**Shell Side**
Stream In	S-118	STEAM5
Stream Out	S-119	STEAM6
Flow Rate (lb/hr)	48,596	4,505
Inlet Temperature (°F)	86	494
Outlet Temperature (°F)	400	494
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	1
	Length (ft)	20
	Surface Area (ft^2)	182
	Tube pitch (in)	1.25
	ΔTlm (°F)	214
	Heat Duty (Btu/hr)	3,515,440
	Total weight (lb)	2,200
	Construction Materials (Shell/Tube)	Carbon Steel/Stainless Steel
Purchase Cost	$ 113,536	
Bare Module Cost	$ 359,910	
Utilities (USD/yr):	$ 4,505	

Heat Exchanger		
Identification	Item:	Heat Exchanger
	Item No:	HX-107
	No. Req'd:	1
Function	Cools product stream before storage	
Operation	Continuous	
Type	Floating Head	
	Tube Side	**Shell Side**
Stream In	S-127	CW 11
Stream Out	S-128	CW 12
Flow Rate (lb/hr)	25,286	123,734
Inlet Temperature (°F)	415	75
Outlet Temperature (°F)	100	95
Design Data:	Number of Tubes	1
	Outer Tube Diameter (in)	4.5
	Length (ft)	16
	Surface Area (ft^2)	314
	Tube pitch (in)	5.6
	ΔTlm (°F)	256
	U (Btu/hr- ft^2-oF)	
	Heat Duty (Btu/hr)	2,476,950
	Total weight (lb)	2,900
	Construction Materials (shell/tube)	Carbon Steel/Stainless Steel
Purchase Cost	$ 27,077	
Bare Module Cost	$ 85,834	
Utilities (USD/yr):	$ 14,759	

Heat Exchanger			
Identification	Item:	Condenser	
	Item No:	D-101-C	
	No. Req'd:	1	
Function	Condense distillate product at the top of D-101		
Operation	Continuous		
Type	Fixed Head Shell and Tube Partial Condenser		
	Tube Side	Shell Side	
Stream In	S-C-1	CW3	
Stream Out	S-C-2	CW4	
Flow Rate (lb/hr)	24,750	2,931,977	
Design Data:	Surface Area per Shell (ft^2)		1,925
	Number of Shells		1
	Shell Diameter (in)		27
	Shell Length (ft)		20
	Tube Material/Shell Material		Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)		1
	Tube Length (ft)		20
	Tube Pitch (in)		1.25
	Shell Material		Carbon Steel
	Total Weight (lb)		14,000
	Heat Duty (BTU/hr)		58,692,479
Purchase Cost	$	109,459	
Bare Module Cost	$	351,363	
Utilities (USD/yr):	$	349,725	

Heat Exchanger		
Identification	Item:	Reboiler
	Item No:	D-101-REB
	No. Req'd:	1
Function	Revaporize the bottoms product of D-101	
Operation	Continuous	
Type	U-Tube Kettle Reboiler	
	Tube Side	**Shell Side**
Stream In	S-R-1	DOWTHERM-3
Stream Out	S-R-2	DOWTHERM-4
Flow Rate (lb/hr)	23,846	391,263
Design Data:	Surface Area per Shell (ft^2)	2,729
	Number of Shells	7
	Shell Diameter (in)	67
	Shell Length (ft)	13
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	211,400
	Heat Duty (BTU/hr)	54,062,820
Purchase Cost	$ 1,312,882	
Bare Module Cost	$ 4,214,351	
Utilities (USD/yr):	DOWTHERM	

Heat Exchanger		
Identification	Item:	Partial Condenser
	Item No:	D-102-C
	No. Req'd:	1
Function	Condense distillate product at the top of D-102	
Operation	Continuous	
Type	Fixed Head Shell and Tube Partial Condenser	
	Tube Side	**Shell Side**
Stream In	S-C-3	CW5
Stream Out	S-C-4	CW6
Flow Rate (lb/hr)	19,472	2,763,294
Design Data:	Surface Area per Shell (ft^2)	2003
	Number of Shells	1
	Shell Diameter (in)	27
	Shell Length (ft)	20
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	14,300
	Heat Duty (BTU/hr)	55,315,822
Purchase Cost	$ 112,282	
Bare Module Cost	$ 360,425	
Utilities (USD/yr):	$ 329,605	

Heat Exchanger		
Identification	Item:	Reboiler
	Item No:	D-102-REB
	No. Req'd:	1
Function	Revaporize the bottoms product of D-102	
Operation	Continuous	
Type	U-Tube Kettle Reboiler	
	Tube Side	**Shell Side**
Stream In	S-R-3	STEAM5
Stream Out	S-R-4	STEAM6
Flow Rate (lb/hr)	5,278	58,243
Design Data:	Surface Area per Shell (ft^2)	2,581
	Number of Shells	5
	Shell Diameter (in)	66
	Shell Length (ft)	13
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	103,000
	Heat Duty (BTU/hr)	51,760,761
Purchase Cost	$ 766,632	
Bare Module Cost	$ 2,460,889	
Utilities (USD/yr):	$ 3,925,547	

Heat Exchanger			
Identification	Item:	Partial Condenser	
	Item No:	D-103-C	
	No. Req'd:	1	
Function	Condense distillate product at the top of D-103		
Operation	Continuous		
Type	Fixed Head Shell and Tube Partial Condenser		
	Tube Side	**Shell Side**	
Stream In	S-C-5	CW7	
Stream Out	S-C-6	CW8	
Flow Rate (lb/hr)	3,809	470,853	
Design Data:	Surface Area per Shell (ft^2)		341
	Number of Shells		1
	Shell Diameter (in)		12
	Shell Length (ft)		20
	Tube Material/Shell Material		Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)		1
	Tube Length (ft)		20
	Tube Pitch (in)		1.25
	Shell Material		Carbon Steel
	Total Weight (lb)		3,200
	Heat Duty (BTU/hr)		9,425,587
Purchase Cost	$ 29,064		
Bare Module Cost	$ 93,295		
Utilities (USD/yr):	$ 56,163		

Heat Exchanger		
Identification	Item:	Reboiler
	Item No:	D-103-REB
	No. Req'd:	1
Function	Revaporize the bottoms product D-103	
Operation	Continuous	
Type	U-Tube Kettle Reboiler	
	Tube Side	**Shell Side**
Stream In	S-R-5	STEAM7
Stream Out	S-R-6	STEAM8
Flow Rate (lb/hr)	1,469	11,572
Design Data:	Surface Area per Shell (ft^2)	962
	Number of Shells	1
	Shell Diameter (in)	40
	Shell Length (ft)	13
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	10,600
	Heat Duty (BTU/hr)	9,030,477
Purchase Cost	$ 74,855	
Bare Module Cost	$ 240,285	
Utilities (USD/yr):	$ 1,121,969	

Heat Exchanger		
Identification	Item:	Partial Condenser
	Item No:	D-104-C
	No. Req'd:	1
Function	Condense distillate product at the top of D-104	
Operation	Continuous	
Type	Fixed Head Shell and Tube Partial Condenser	
	Tube Side	**Shell Side**
Stream In	S-C-7	CW9
Stream Out	S-C-8	CW10
Flow Rate (lb/hr)	5,653	608,848
Design Data:	Surface Area per Shell (ft^2)	507
	Number of Shells	1
	Shell Diameter (in)	14
	Shell Length (ft)	20
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	4,100
	Heat Duty (BTU/hr)	12,187,883
Purchase Cost	$ 36,695	
Bare Module Cost	$ 117,791	
Utilities (USD/yr):	$ 72,623	

Heat Exchanger		
Identification	Item:	Reboiler
	Item No:	D-104-REB
	No. Req'd:	1
Function	Revaporize the bottoms product D-104	
Operation	Continuous	
Type	U-Tube Kettle Reboiler	
	Tube Side	**Shell Side**
Stream In	S-R-7	DOWTHERM-5
Stream Out	S-R-8	DOWTHERM-6
Flow Rate (lb/hr)	13,819	385,000
Design Data:	Surface Area per Shell (ft^2)	157
	Number of Shells	1
	Shell Diameter (in)	18
	Shell Length (ft)	13
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
	Tube Outside Diameter (in)	1
	Tube Length (ft)	20
	Tube Pitch (in)	1.25
	Shell Material	Carbon Steel
	Total Weight (lb)	2,100
	Heat Duty (BTU/hr)	1,380,582
Purchase Cost	$ 21,327	
Bare Module Cost	$ 68,460	
Utilities (USD/yr):	DOWTHERM	

Pump

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	P-101
	No. Req'd:	2
Function	Pressurizes stream entering D-101	
Operation	Continuous	
Type	Centrifugal	
Materials Handled:	**Stream In:**	**Stream Out:**
	S-116	S-117
Flow Rate (lb/hr)	48,596	48,596
Temperature (°F)	86	86
Pressure (psia)	25	150
Design Data:	Density of Fluid (lb/cuft)	60
	Brake Power (hp)	14
	Pump Head (ft)	302
	Consumed Power (BTU/hr)	35,077
	Pump Efficiency	0.54
	Construction Material	Stainless Steel
Purchase Cost:	$ 22,373	
Bare Module Cost:	$ 73,830	
Utilities (USD/yr):	$ 5,616	
Comments	1 Pump for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	P-102
	No. Req'd:	2
Function	Sends acrylic acid through pipeline to storage tank	
Operation	Continuous	
Type	Centrifugal	
Materials Handled:		
	Stream In:	**Stream Out:**
	S-128	PRODUCT
Flow Rate (lb/hr)	25,286	25,314
Temperature (°F)	100	100
Pressure (psia)	63	75
Design Data:	Density of Fluid (lb/cuft)	58
	Brake Power (hp)	0.79
	Pump Head (ft-lb_f/lb_m)	27
	Consumed Power (BTU/hr)	11
	Pump Efficiency	0.44
	Construction Material	Stainless Steel
Purchase Cost:	$ 5,645	
Bare Module Cost:	$ 18,629	
Utilities (USD/yr):	$ 320	
Comments	1 Pump for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	P-103
	No. Req'd:	40
Function	Moves Dowtherm through cooling/heating loop	
Operation	Continuous	
Type	Centrifugal	
Materials Handled:	**Stream In:**	**Stream Out:**
	DOWTHERM	DOWTHERM
Flow Rate (lb/hr)	25,314	25,314
Temperature (°F)	198	1983
Pressure (psia)	15	40
Design Data:	Density of Fluid (lb/cuft)	50
	Brake Power (hp)	15,764
	Pump Head (ft-lb_f/lb_m)	1,037
	Consumed Power (kW)	574
	Pump Efficiency	0.83
	Construction Material	Stainless Steel
Purchase Cost:	$ 53,504	
Bare Module Cost:	$ 171,748	
Utilities (USD/yr):	$ 313,789	
Comments	20 pumps for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	D-101-P
	No. Req'd:	2
Function	Pump that recycles reflux into top of D-101	
Operation	Continuous	
Type	Centrifugal	
Design Data:	Flow Rate (gpm)	238
	Temperature (°F)	368
	Pressure (psia)	120
	Brake Power (hp)	20
	Pump Head (ft-lb_f/lb_m)	225
	Construction Material	Stainless Steel
Purchase Cost:	$ 9,305	
Bare Module Cost:	$ 30,707	
Utilities (USD/yr):	$ 8,150	
Comments	1 Pump for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	D-102-P
	No. Req'd:	2
Function	Pump that recycles reflux into top of D-102	
Operation	Continuous	
Type	Centrifugal	
Design Data:	Flow Rate (gpm)	200
	Temperature (°F)	345
	Pressure (psia)	80
	Brake Power (hp)	15
	Pump Head (ft-lb_f/lb_m)	225
	Construction Material	Stainless Steel
Purchase Cost:	$ 8,573	
Bare Module Cost:	$ 28,291	
Utilities (USD/yr):	$ 8,150	
Comments	1 Pump for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	D-103-P
	No. Req'd:	2
Function	Pump that recycles reflux into top of D-103	
Operation	Continuous	
Type	Centrifugal	
Design Data:	Flow Rate (gpm)	30
	Temperature (°F)	348
	Pressure (psia)	75
	Brake Power (hp)	3
	Pump Head ($ft\text{-}lb_f/lb_m$)	225
	Construction Material	Carbon Steel
Purchase Cost:	$ 6,377	
Bare Module Cost:	$ 21,044	
Utilities (USD/yr):	$ 8,150	
Comments	1 Pump for backup	

Pump		
Identification	Item:	Centrifugal Pump
	Item No:	D-104-P
	No. Req'd:	2
Function	Pump that recycles reflux into top of D-104	
Operation	Continuous	
Type	Centrifugal	
Design Data:	Flow Rate (gpm)	60
	Temperature (°F)	315
	Pressure (psia)	75
	Brake Power (hp)	5
	Pump Head (ft-lb_f/lb_m)	225
	Construction Material	Stainless Steel
Purchase Cost:	$ 6,586	
Bare Module Cost:	$ 21,734	
Utilities (USD/yr):	$ 8,150	
Comments	1 Pump for backup	

Reactor

Reactor		
Identification	Item: Item No: No. Req'd:	Reactor R-101 1
Function **Operation** **Type**	Converts Propane to Acrylic Acid Continuous Catalyst-Packed Shell and Tube Heat Exchanger	
Materials Handled:	**Stream In:** S-107	**Stream Out:** S-108
Flow Rate (lb/hr)	620,230	620,230
Temperature (°F)	740	780
Pressure (psia)	50	44
Composition (mass frac)		
Propane	0.291	0.262
Propylene	0.031	0.032
Oxygen	0.047	0.004
Water	0.012	0.036
Carbon Dioxide	0.094	0.097
Nitrogen	0.521	0.521
Acetic Acid	0.001	0.002
Acrylic Acid	0.003	0.046

Reactor Continued

Design Data:	Catalyst	$Mo_1V_{0.3}Te_{0.23}Nb_{0.125}O_x$
	Catalyst Loading (lb)	160
	Inert (ft^3)	30
	Number of Tubes	4,000
	Tube Diameter (in)	2
	Surface Area	16,755
	Length (ft)	8
	Reactor Volume (ft^3)	698
	Space Velocity (hr-1)	1,662
	Residence Time (sec)	2
	Bed Porosity	0.4
	Pressure Drop (psia)	6
	Heat Duty (BTU/hr)	120,000,000
	Coolant (Shell Side)	Dowtherm A
	Coolant Flow Rate (lb/hr)	385,000
	Coolant In	DOWTHERM-1
	Coolant Inlet Temperature (°F)	198
	Coolant Out	DOWTHERM-2
	Coolant Outlet Temperature (°F)	738
	Tube Material/Shell Material	Stainless Steel/Carbon Steel
Reactor Purchase Cost	$ 281,389	
Total Bare Module Cost	$ 903,259	
Catalyst Cost	$ 697,093	
Comments	Catalyst should be replaced every 2 years	

Storage Tanks

Storage Tank		
Identification	Item:	Reflux Accumulator
	Item No:	D-101-RA
	No. Req'd:	1
Function	Accumulates the reflux in D-101	
Operation	Continuous	
Type	Horizontal Vessel	
Design Data:	Pressure (psia)	120
	Temperature (°F)	368
	Diameter (ft)	4.5
	Length (ft)	13.5
	Storage Volume (ft^3)	215
	Material Thickness (in)	0.25
	Construction Material	Carbon Steel
Purchase Cost:	$ 37,636	
Bare Module Cost:	$ 120,813	

Storage Tank		
Identification	Item:	Reflux Accumulator
	Item No:	D-102-RA
	No. Req'd:	1
Function	Accumulates the reflux in D-102	
Operation	Continuous	
Type	Horizontal Vessel	
Design Data:	Pressure (psia)	95
	Temperature (°F)	345
	Diameter (ft)	4
	Length (ft)	12.5
	Storage Volume (ft^3)	157
	Material Thickness (in)	0.188
	Construction Material	Carbon Steel
Purchase Cost:	$ 28,645	
Bare Module Cost:	$ 91,950	

Storage Tank		
Identification	Item:	Reflux Accumulator
	Item No:	D-103-RA
	No. Req'd:	1
Function	Accumulates the reflux in D-103	
Operation	Continuous	
Type	Horizontal Vessel	
Design Data:	Pressure (psia)	90
	Temperature (°F)	348
	Diameter (ft)	3
	Length(ft)	3.5
	Storage Volume (ft^3)	25
	Material Thickness (in)	0.19
	Construction Material	Stainless Steel
Purchase Cost:	$ 17,459	
Bare Module Cost:	$ 56,043	

Storage Tank		
Identification	Item:	Reflux Accumulator
	Item No:	D-104-RA
	No. Req'd:	1
Function	Accumulates the reflux in D-104	
Operation	Continuous	
Type	Horizontal Vessel	
Design Data:	Pressure (psia)	90
	Temperature (°F)	314
	Diameter (ft)	3
	Length(ft)	6.5
	Storage Volume (ft^3)	46
	Material Thickness (in)	0.19
	Construction Material	Stainless Steel
Purchase Cost:	$ 19,863	
Bare Module Cost:	$ 63,760	

Storage Tank		
Identification	Item:	Storage Tank
	Item No:	PropaneStorage
	No. Req'd:	1
Function	Stores emergency supply of propane feed	
Operation	Continuous	
Type	Horizontal Vessel	
Design Data:	Pressure (psia)	165
	Temperature (°F)	75
	Diameter (ft)	10
	Length(ft)	50
	Storage Volume (ft^3)	6120
	Material Thickness (in)	0.97
	Construction Material	Carbon Steel
Purchase Cost:	$ 168,131	
Bare Module Cost:	$ 512,797	
Comments	Stores 8 hours of propane feed	

Storage Tank		
Identification	Item:	Storage Tank
	Item No:	ProductStorage
	No. Req'd:	1
Function	Stores produced acrylic acid	
Operation	Continuous	
Type	Cone Roof	
Design Data:	Pressure (psia)	15
	Temperature (°F)	75
	Storage Volume (ft^3)	700000
	Construction Material	Stainless Steel
Purchase Cost:	$ 291,705	
Bare Module Cost:	$ 291,705	
Comments	Stores 1 weeks’ worth of acrylic acid produced	

Turbine

Turbine			
Identification	Item:		Turbine
	Item No:		T-101
	No. Req'd:		1
Function	Expands feed oxygen from pressurized pipeline		
Operation	Continuous		
Type	N/A		
Materials Handled:			
	Stream In:		**Stream Out:**
	O2		S-100
Flow Rate (lb/hr)		23,839	23,839
Temperature (°F)		75	-106
Pressure (psia)		500	60
Design Data:	Number of Stages		1
	Isentropic Efficiency		0.72
	Total work (hp)		-345
	Material of Construction		Carbon Steel
Purchase Cost:	$	176,055	
Bare Module Cost	$	565,135	
Utilities (USD/yr):		N/A	

Section 7

Energy Balance & Utility Requirements

Heat Integration Strategy

Heat integration techniques were used in order to reduce the net utilities requirements. The reactor effluent, which is at 780°F, is used to heat the feed to the reactor. The effluent transfers about 100,000,000 BTU/hr to the reactor feed (S-107), which takes the feed from 358°F to 740°F. Not only does this reduce the utilities needed to heat the feed, but it also reduces the utilities needed to cool the effluent before it enters the flash drum at standard ambient temperature.

Additionally, the Dowtherm stream that is used to remove heat from the reactor is used as a heat source in two reboilers and a heater. The Dowtherm leaves the reactor and travels to the reboiler of tower D-101, to the reboiler of tower D-104, and finally to HX-105. Upon exiting the shell side of this heater, the Dowtherm enters a network of pumps, which send it back to cool the reactor. More details for the Dowtherm cooling loop can be found in the Dowtherm utility section below.

As a result of both these heat integration strategies, steam and cooling water requirements were significantly reduced, creating an overall more efficient process and decreasing operating costs.

Work Integration Strategy

In an effort to reduce electricity consumption, the work generated by expanding the inlet oxygen through a turbine (T-101) was used to partially offset the electricity required by the air compressor (C-102).

Table 7.1: T-101 Electricity Savings

T-101 Electricity Savings		
C-102 Electricity Requirement	298	kW
T-101 Electricity Requirement	-257	kW
Net Electricity Required	41	kW
Electricity Saved	257	kW
Savings	$141,000.00	/yr
Cost of T-101	$378,500.00	
Payback Period	2.7	yrs
ROI	37%	

By using the oxygen expansion to generate electricity, $141,000 of savings is realized. Therefore, the $378,500 investment in the turbine has a payback period of 2.7 years and a return on investment (ROI) of approximately 37%.

Cooling Water

This process requires 1,206,307 gal/hr of cooling water to cool and condense process streams in various condensers. Cooling water is available at $0.125/1,000 gal, adjusted for 2012 prices. Cooling water is assumed to enter the plant at 75°F and 50 psia and exit at 95°F. At 95°F, the used cooling water is dischargeable without any further processing. Total cooling water costs are $1,198,587 annually, which is 7% of the total utilities costs.

Steam

This process requires 66,127 lb/hr of 100 psia steam and 16,076 lb/hr of 400 psia steam. The low-pressure steam is available at $8.50/1,000 lb and the high-pressure steam is available at $12.20/1,000 lb, adjusted for 2012 prices. About 88% of the low-pressure steam is used in the reboiler of tower D-102 and about 72% of the high-pressure steam is used in the reboiler of tower D-103. The high-pressure steam is used to heat streams to higher temperatures which the low-pressure steam cannot attain because its operating temperature is too low. The annual cost of the 100 psia steam is $4,456,928 and the annual cost for the 400 psia steam is $1,558,735, which represent 26% and 9% of the total utilities cost respectively.

Electricity

This process requires 18,526 kW of electricity to power compressors and pumps. Electricity is available at $0.069/kWh, adjusted for 2012 prices. The pumps (P-103) in the Dowtherm cooling/heating cycle use about 62% of the total electricity and the recycle stream compressor (C-101) uses about 37%. The annual cost for electricity is $10,124,034, which represents 58% of the total utilities cost.

Dowtherm A

Dowtherm A is used to cool the reactor and serves as a heat source for two reboilers and a heater in the process. A mass flow rate of 385,000 lb/hr is required to sufficiently cool the reactor assuming the Dowtherm is allowed to heat up by 300°F. This still maintains the assumed log-mean temperature difference of 100 degrees Fahrenheit across the fixed bed reactor, which was used to calculate the required heat exchange surface area for sizing purposes. Upon exiting the reactor the Dowtherm enters D-101-REB, then HX-105, and finally D-104-REB. After exiting this final reboiler, it enters a network of pumps that keep it cycling through this heat exchange loop. It is assumed that after the Dowtherm exits D-104-REB at 203°F it cools back down to 198°F due to heat losses in the pipes carrying it. The Dowtherm process requires a network of 20 pumps in parallel, each which consume about 575 kW of electricity. In total, the annual operating cost of the pumps is $6,276,000. While this is significant, the savings realized by using the Dowtherm as a heating source justify the expense.

Using the Dowtherm cooling/heating loop, the net utilities savings is $4,000,000 annually, while the total fixed cost of the Dowtherm chemical and the required pumps is $7,570,000. This gives a payback period of just under 2 years and a return on investment of 53%.

Table 7.2: Dowtherm Utilities Savings

Dowtherm Utilities Savings		
Utilities Savings	$10,285,000.00	
Variable Cost of Electricity for Pumps	$6,276,000.00	
Net Savings	$4,000,000.00	
Fixed Cost of Pumps	$6,870,000.00	
Fixed Cost of Dowtherm	$699,530.00	
Total Fixed Cost	$7,570,000.00	
Payback Period	1.9	yrs
ROI	53%	

Table 7.3: Dowtherm Cooling/Heating Loop

Dowtherm Cooling/Heating Loop		
Mass Flow Rate	385,000	lb/hr
Specific Heat	2.249	Btu/kg-K
Cost	$699,530.00	
Reactor		
Heat Duty	118,000,000	Btu/hr
Dowtherm Inlet Temperature	198	F
Dowtherm Exit Temperature	738	F
D-101-reb		
Heat Duty	54,100,000	Btu/hr
Dowtherm Inlet Temperature	738	F

Dowtherm Exit Temperature	458	F
HX-105		
Heat Duty	27,900,000	Btu/hr
Dowtherm Inlet Temperature	458	F
Dowtherm Exit Temperature	299	F
D-104-reb		
Heat Duty	13,800,000.00	Btu/hr
Dowtherm Inlet Temperature	299	F
Dowtherm Exit Temperature	203	F

Table 7.4: Utility Requirements and Costs

Utility Requirements and Costs			
Cooling Water	**Flow (gal/hr)**	**Cost (USD/hr)**	**Cost (USD/yr)**
HX-104	378,131.00	$47.44	$375,710.96
HX-107	14,854.00	$1.86	$14,758.93
D-101-cond	351,978.00	$44.16	$349,725.34
D-102-cond	331,728.00	$41.62	$329,604.94
D-103-cond	56,525.00	$7.09	$56,163.24
D-104-cond	73,091.00	$9.17	$72,623.22
Total	1,206,307.00	$151.34	$1,198,586.64

Steam at 100 psi	**Flow (lb/hr)**	**Cost (USD/hr)**	**Cost (USD/yr)**
D-102-reb	58,243.23	$495.65	$3,925,547.31
HX-101	1,998.22	$17.00	$134,678.30
HX-102	5,885.86	$50.09	$396,702.53
Total	66,127.32	$562.74	$4,456,928.14
Steam at 400 psi	**Flow (lb/hr)**	**Cost (USD/hr)**	**Cost (USD/yr)**
D-103-reb	11,571.60	$141.66	$1,121,968.55
HX-106	4,504.67	$55.15	$436,766.91
Total	16,076.27	$196.81	$1,558,735.46
Electricity	**kW**	**Cost (USD/hr)**	**Cost (USD/yr)**
C-101	6,930.50	$478.20	$3,787,379.64
C-102	40.88	$2.82	$22,341.63
P-101	10.28	$0.71	$5,615.90
P-102	0.59	$0.04	$320.02
D-101-P	14.91	$1.03	$8,150.20
D-102-P	14.91	$1.03	$8,150.20
D-102-P	14.91	$1.03	$8,150.20
D-104-P	14.91	$1.03	$8,150.20
P-103 (x20)	11,484.00	$792.40	$6,275,776.32
Total	18,525.90	$1,278.29	$10,124,034.32

Section 8

Other Important Considerations

8.1 Plant Location & Start-Up

The plant should be located in the Gulf Coast region in order to capitalize on the proximity and abundance of propane supply produced from shale gas refining. For other locations, a site factor may apply to adjust for the additional costs of raw materials and transportation. Due to the use of cooling water throughout the process, the plant should be located as close to a large body of water as possible. In addition, the layout of the plant should be carefully planned in order to separate units that may interfere. The reactor should be isolated from all storage tanks to prevent explosion in the event of a temperature rise. The main process compressor (C-101) is likely to generate a large amount of noise and vibration, and should be placed carefully.

Prior to plant start-up, air should be pumped through the system before decompressed oxygen in order to ensure there is enough inert (nitrogen) to block the flammability limits of the oxygen/propane system. As the system reaches steady state, the control systems should limit the amount of decompressed oxygen being pumped to ensure a fuel-rich reactant stream.

The plant utilizes many heat exchangers to preheat and cool streams, which can pose a major challenge to startup. Namely, HX-103, R-101, HX-105, D-104-REB, and D-101-REB are all affected by the lack of reaction heat prior to steady state. In addition, Dowtherm A must also be heated up to the minimum temperature (198°F) for the designed cooling system. Secondary heat sources, such as pressurized steam, must be used initially to raise the temperature of the reactor system and in place of the Dowtherm A heating systems.

8.2 Transportation & Storage

The propane and pressurized O_2 will come from a pipeline already existing within the industrial complex. Eight hours' worth of propane will be stored in a storage tank, PropaneStorage, in order to prevent minor shut downs of the process due to supplier or pipeline problems. If a larger plant shut down is needed, the process can be placed on recycle.

Storage and shipment temperatures of acrylic acid should be kept in the range of 59°F to 77°F and under atmospheric pressure with air to prevent undesired reactions. A weeks' worth of acrylic acid will be stored in a storage tank, ProductStorage. However, the polymerization of acrylic acid is very violent and may auto ignite. Thus, it is important to inhibit polymerization with a stabilizer such as hydroquinone monomethyl ether (MEHQ) and prevent storage tanks from being exposed to high temperature. As oxygen is necessary to activate MEHQ, it is important to maintain a gas mixture of at least 5% to 21% by volume of oxygen.

Similarly, acrylic acid being loaded into drums, rail cars, or tank trucks must have a dissolved oxygen concentration equivalent to saturation with one atmosphere of gas containing 5% to 21% by volume oxygen. Residues in transfer lines should be blown out with the same gas mixture composition. Acrylic acid will be transported offsite to customers through a railcar system. Assuming the capacity of each railcar to be 20,000 gallons, four railcars will be used to transport 70,000 gallons of acrylic acid offsite to consumers each day. If consumers are onsite, a direct transfer feed line will be attached and reduce transportation and delivery costs.

8.3 Process Controllability

Exothermic oxidation reactions such as that used in this process run the risk of causing runaway reactors when not controlled properly. This reactor uses oxygen as a limiting reagent and feeds propane in a stochiometric excess. Doing this accomplishes the dual purposes of mitigating the risk of a runaway reactor and limiting the conversion of propane to the order of 10%, which increases the selectivity of acrylic acid formation. The temperature of the reactor will be managed by using a stable chemical product, Dowtherm, flowing counter-currently with reactor contents, arranged in a shell-tube heat exchanger as described in Section 5. If the temperature of the reactor needs further control, the ratio of catalyst beads to inert beads can be adjusted. This would reduce the speed of the reaction and result in a more favorable temperature profile because the Dowtherm could remove more heat.

8.4 Maintenance and Emergency Procedures

Proper equipment maintenance is vital for ensuring that unforeseen stoppages in production are minimized. The process simulation assumes that the plant is operational at full capacity for 330 days a year to account for routine maintenance. Should any equipment fail unexpectedly, the profitability of the plant will be dramatically affected by halting revenues while expensive equipment and labor remain idle. Avoiding this requires a mixture of corrective and preventative maintenance, as well as careful condition-based maintenance procedures, as outlined by WIPRO Technologies.[16] The reactor walls should be periodically inspected for signs of corrosion or heat damage. The catalyst packing must also be inspected regularly, and may need to be regenerated if the active surface area decreases. It is estimated that the catalyst life will be approximately 2 years. Pumps and compressors should be closely monitored for signs of performance losses and physical damage. The cost of back-ups for all liquid pumps used in this process are included in the economic analysis should any of the pumps fail unexpectedly. The distillation columns, along with all associated reboilers, condensers, pumps, and trays, should be monitored for signs of wear and reduced performance. Operators must check the integrity of all piping to avoid leaks and blockages, and the piping systems may need to be flushed with inert periodically to prevent build-up.

In the event of an emergency, the process contains control valves that can be closed to prevent the flow of feed to the reactor, product to various stages of the separation process, or recycle gases to the feed mixture. In addition, the power can be cut to all of the compressors and pumps to halt the process. Should the reactor near the auto-ignition temperatures discussed in *Safety and Health Considerations*, operators should seek refuge outside and away from the concrete reactor containment unit. Proper fire extinguishers, flame retardant materials, and safety procedures should be implemented according to all building and industrial codes.

[16] Padmanabhan, H. Condition Based Maintenance Of Rotating Equipments on OSI PI Platform - Refineries/Petrochem Plants: Wipro Council for Industry Research.

8.5 Process Safety and Health Concerns

This process involves the selective oxidation of a gaseous hydrocarbon, meaning that the primary safety concern is the possibility for explosion. As a result, great care has been taken to ensure that all streams in the process are safely outside the flammability limits of propane. The process is controlled primarily by running under an excess of propane, making oxygen the limiting reagent. The stream feeding the reactor contains the most oxygen in the process (aside from the pure oxygen feed), and is 21.8% propane and only 4.6% oxygen, with the majority of the stream being inert nitrogen at 61.6%. The Upper Flammability Limit (UFL) of propane is 10.1% in air and 55% in pure oxygen. All streams are thus too oxygen-poor to allow combustion to occur. It should be noted that all three mixers in the process (M-101, M-102, and M-103) should be carefully monitored and isolated from all flames and sparks, as their contents may pass through the flammable regime as they mix recycled propane with air and pure oxygen feeds.

Another safety concern is the presence of high temperatures during the process. The optimal reaction temperature is 750°F, and the reactor outlet temperature could rise as high as 780°F even with cooling with molten salts. This is still well under the auto-ignition temperature of propane and propylene (878°F and 858°F, respectively). In the unlikely event that the reactor temperature begins to approach these values, a control valve upstream from the reactor (V-101) could be closed to stop the flow of feed so that the reactor may cool. Still, it is recommended that a concrete shell be erected over the reactor in order to keep operators safe in the event of a fire or explosion. Care must be taken to ensure propane does not leak from the reactor into this shell, where it may form a combustible mixture. The Occupational Safety and Health Administration recommends using Detector Tubes manufactured by AUER/MSA or Drager in order to detect concentrations greater than 200 ppm of propane in the air.[17]

The process also involves storage of liquefied propane and acrylic acid to account for changes in supply of propane from the pipeline and demand for acrylic acid. It is recommended that the propane storage tank be stored in a pressure vessel so as to prevent explosive vapor from forming. In addition, the propane storage tank must be isolated from all sparks and flames, and operators must be careful to check for leaks using the methods described above. The acrylic acid storage tank can be designed as a fixed cone roof because acrylic acid will have a relatively low vapor pressure at storage conditions.

[17] U.S. Department of Labor. Propane. http://www.osha.gov/dts/chemicalsampling/data/CH_264000.html

8.6 Environmental Considerations

Acrylic acid is relatively non-toxic to bacteria and soil microorganisms. It is also miscible with water and is not expected to adsorb significantly in soil or sediment. When released into the atmosphere, it reacts to produce hydroxyl radicals and ozone which results in quick degradation. There is no bioaccumulation of acrylic acid as it readily biodegrades in water and has an atmospheric lifetime of less than one month.[18]

Environmental concerns will be analyzed with respect to U.S. standards for pollution control. As there is no solid waste emitted from this process, the plant will meet the Federal Hazardous and Solid Waste Amendments (HWSA) under the Resource Conservation and Recovery Act (RCRA).

The problematic pollutants for this process in terms of air quality are CO_x. Currently, the EPA's Clean Air Act only regulates CO at the level of 35 ppm per hour.[19] As this process assumes that all CO is quickly oxidized to CO_2, only trace amounts of CO may remain and this standard will easily be met. Although there is no present standard for CO_2 emissions, companies are required to obtain permits for construction and operation of their facilities from the EPA to insure compliance.[20] Additionally, CO_2 emissions are likely to be regulated in the future. The process may need to include a carbon capture and sequestration process if the plant is found to be above regulatory limits at a future date.

The main impact on the environment is through the organic content in the wastewater streams. A cost for wastewater treatment has been included in the financial calculations and an off-site facility is assumed.

[18] World Health Organization: International Programme on Chemical Safety. (1997). Environmental Health Criteria 191: Acrylic Acid.
[19] Environmental Protection Agency (2012). National Ambient Air Quality Standards (NAAQS) http://www.epa.gov/air/criteria.html
[20] Haggin, P. (2012). EPA's CO2 Regulation Upheld as "Unambiguously Correct". Time. http://science.time.com/2012/06/28/epas-co2-regulation-upheld-as-unambiguously-correct/

Section 9

Cost Summaries

9.1 Fixed Capital Summary

Table 9.1: Fixed Capital Investment Summary

Bare Module Costs	
Process Machinery	$41,454,717
Spares	$3,629,192
Storage	$831,406
Other Equipment	$699,530
Catalysts	$5,576,741
Computers, Software, Etc.	-
Total Bare Module Costs:	$52,191,590
Plus: Cost of Site Preparations	$2,609,579
Plus: Cost of Service Facilities	$2,609,579
Plus: Allocated Costs for utility plants and related facilities	-
Direct Permanent Investment	$57,410,744
Plus: Cost of Contingencies & Contractor Fees	$10,333,934
Total Depreciable Capital	$67,744,678
Plus: Cost of Land	$1,354,894
Plus: Cost of Royalties	-
Plus: Cost of Plant Start-Up	$6,774,468
Total Unadjusted Permanent Investment	$75,874,040
Site Factor	1.0
Total Permanent Investment	**$75,874,040**

Purchase costs and bare module costs of equipment were estimated using Aspen IPE and Aspen Economic Analyzer. Once total bare module costs were estimated, cost of site preparation and service facilities were estimated as 5% of total bare module costs using the method described in Seider, Seader, Lewin, and Widago. It was assumed that there were already existing utility and wastewater treatment plants available so the allocated costs for utility plants and related facilities was assumed to be zero. Also following the procedure outline in Seider et al, the cost of contingencies and contractor fees was estimated to be 18% of direct permanent investment, the cost of land is 2% of total depreciable capital, and plant start-up cost is estimated to be 10% of total depreciable capital.

Table 9.2: Total Capital Investment Summary

Total Permanent Investment:	$75,874,040
Plus: Present Value of 2014 Working Capital	$13,228,811
Plus: Present Value of 2015 Working Capital	$5,751,657
Plus: Present Value of 2016 Working Capital	$5,001,441
Total Capital Investment	**$99,855,948**

The total capital investment, depicted in Table 9.2, includes total permanent investment and the net present value of working capital contributions. The working capital forms a significant part of the total capital investment of approximately 24%.

9.2 Variable Cost Summary

Table 9.3: Variable Cost Summary

General Expenses				
Selling/ Transfer Expenses:				$10,500,000
Direct Research:				$16,800,000
Allocated Research:				$1,750,000
Administrative Expense:				$7,000,000
Management Incentive Compensation:				$4,375,000
Total General Expenses				$40,425,000
Raw Materials				
Propane				$42,600,000
Compressed Oxygen				$6,000,000
Total Raw Materials				$48,600,000
Byproducts				
Wastewater Treatment				$7,564,660
Total Byproducts				$7,564,660
Utilities				
High Pressure Steam				$2,440,000
Low Pressure Steam				$1,658,945
Cooling Water				$25,000
Electricity				$13,800,000
Total Utilities				$17,136,845
Total Variable Cost				$113,726,505

General expenses cover expenses associated with the direct management of product within the plant but are not related to the direct manufacturing cost. Instead, they are assumed to be a fixed percentage of sales.[21]

[21] Seider, W. D., Seader, J. D., Lewin, D. R., & Widagdo, S. (2009). Product and Process Design Principles: Synthesis, Analysis, and Evaluation (Vol. 3). Hoboken, NJ: John Wiley & Sons, Inc.

9.3 Fixed Cost Summary

Table 9.4: Fixed Cost Summary

Operations				
Direct Wages and Benefits				$2,496,000
Direct Salaries and Benefits				$748,800
Operating Supplies and Services				$149,760
Technical Assistance to Manufacturing				$4,500,000
Control Laboratory				$4,500,000
Total Operations				$12,394,560
Maintenance				
Wages and Benefits				$3,026,807
Salaries and Benefits				$756,702
Materials and Services				$3,026,807
Maintenance Overhead				$151,340
Total Maintenance				$6,961,656
Operating Overhead				
General Plant Overhead				$527,123
Mechanical Department Services				$210,849
Employee Relations Department				$421,699
Business Services				$520,095
Total Operating Overhead				$1,679,766
Property Taxes and Insurance				
Property Taxes and Insurance				$2,017,871
Other Annual Expenses				
Rental Fees:				-
Licensing Fees:				-
Total Fixed Costs				$23,053,854

Fixed costs for the process were estimated according to the methods described in Seider, Seader, Lewin, and Widago. Operations expense was estimated by assuming 6 operators per shift (with 5 shifts), an hourly wage of $40/operator hour, and including 30% of direct wages and benefits. Maintenance expense was estimated by including 4.5% of depreciable capital for wages and benefits, 25% of maintenance wages and benefits for salaries and benefits, 5% of maintenance wages and benefits for maintenance overhead and 100% of maintenance wages and benefits for materials and services. Operating overhead was computed as 7.5% of wages and benefits for general plant overhead, 3% of wages and benefits for mechanical department services, 6% of wages and benefits for employee relations department, and 7.4% of wages and benefits for business services. Property taxes and insurance were estimated as 3% of total depreciable capital. Depreciation is not calculated as an operating expense and instead the MACRS depreciation schedule is used.

9.4 Pricing of Wastewater and Purge Streams

A cost was assigned to the aggregated wastewater stream as a function of the flow rate of water in gpm and the loading of organic compounds. The operating cost of Deep-Tank Activated-Sludge Treatment is \$300/yr·gpm of hydraulic flow plus \$2,000/yr·(lb organic/hr), summing to \$7,564,660 per year with the current waste water stream.[22] The resulting water stream is then considered safe to discharge into the environment. As stated in the project charter, the design and costing of construction of the wastewater facility is considered out of project scope, and the investment costs of the wastewater plant were not calculated.

The lower heating values of propane, propene, acrylic acid, and acetic acid were mass-weighted and used to calculate the resulting heating value of the stream. Approximately 116.1 MM BTU/hr can be released through burning the purge stream. If this stream could be converted to electricity with an assumed 20% efficiency at \$0.16/kWh, the stream is worth approximately \$8.6 million per year. Alternatively, if the same stream could be converted to heat at 50% efficiency at \$0.06/kWh, the stream is worth \$8.1 million. It was determined that it will be more economical to convert the stream to heat in order to avoid the considerable equipment costs of turbines, generators, condensers, and the like that would be required to generate the electricity. The heating value of 116 MM BTU/hr can be deducted from the required energy utility inputs.

[22] Mulholland, K. L., & Dyer, J. A. (1998). Pollution Prevention: Methodology, Technologies and Practices: American Institute of Chemical Engineers.

Section 10

Economic Analysis

10.1 Economic Analysis

The economic analysis of this process was conducted using the discounted cash flow method. Once cash flows for each period were estimated, the net present value (NPV) of the cash flows can be calculated by applying a discount factor to each period's cash flow and taking the sum. For this process, a 15% discount rate was assumed. The discount rate should reflect the perceived risk of the project and the macro-economic exposure inherent in plant operations. Based on this information, a 15% discount rate is reasonably conservative and reflects the high degrees of uncertainty in plant operations, which is consistent with a plant in the first stages of design. Using this discount rate, the NPV is calculated as $384,963,400, over the assumed 20 year life of the plant.

Another metric often used when evaluating different investment opportunities is the internal rate of return (IRR). IRR is the discount rate at which the NPV of a series of cash flows is zero. This is a kind of annualized return on investment. The IRR of this process was calculated to be 84.9%, reflecting a reasonably high return and suggesting that this process warrants further investigation.

Table 10.1: Cash Flow Summary

Cash Flow Summary

Year	Percentage of Design Capacity	Product Unit Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Depletion Allowance	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 15%
2013	0%		-	-	-	-	-	-	-	-	-	-	-	-
2014	0%		-	(75,874,000)	(15,213,100)	-	-	-	-	-	-	-	(91,087,200)	(79,206,200)
2015	45%	$1.75	157,500,000	-	(7,606,600)	(50,267,300)	(23,124,700)	(13,548,900)	-	70,559,000	(26,106,800)	44,452,200	50,394,600	(41,100,700)
2016	68%	$1.75	236,250,000	-	(7,606,600)	(78,417,000)	(24,049,700)	(21,678,300)	-	112,105,000	(41,478,800)	70,626,100	84,697,900	14,589,500
2017	90%	$1.75	315,000,000	-	-	(108,738,200)	(25,011,700)	(13,007,000)	-	168,243,100	(62,249,900)	105,993,100	119,000,100	82,628,200
2018	90%	$1.75	315,000,000	-	-	(113,087,800)	(26,012,200)	(7,804,200)	-	168,095,900	(62,195,500)	105,900,400	113,704,600	139,159,500
2019	90%	$1.75	315,000,000	-	-	(117,611,300)	(27,052,700)	(7,804,200)	-	162,531,900	(60,136,800)	102,395,100	110,199,300	186,801,700
2020	90%	$1.75	315,000,000	-	-	(122,315,700)	(28,134,800)	(3,902,100)	-	160,647,400	(59,439,500)	101,207,900	105,110,000	226,316,400
2021	90%	$1.75	315,000,000	-	-	(127,208,300)	(29,260,200)	-	-	158,531,500	(58,656,700)	99,874,800	99,874,800	258,965,700
2022	90%	$1.75	315,000,000	-	-	(132,296,700)	(30,430,600)	-	-	152,272,800	(56,340,900)	95,931,800	95,931,800	286,235,500
2023	90%	$1.75	315,000,000	-	-	(137,588,500)	(31,647,800)	-	-	145,763,700	(53,932,600)	91,831,100	91,831,100	308,934,800
2024	90%	$1.75	315,000,000	-	-	(143,092,100)	(32,913,700)	-	-	138,994,200	(51,427,900)	87,566,400	87,566,400	327,756,600
2025	90%	$1.75	315,000,000	-	-	(148,815,800)	(34,230,200)	-	-	131,954,000	(48,823,000)	83,131,000	83,131,000	343,294,300
2026	90%	$1.75	315,000,000	-	-	(154,768,400)	(35,599,500)	-	-	124,632,100	(46,113,900)	78,518,300	78,518,300	356,055,700
2027	90%	$1.75	315,000,000	-	-	(160,959,100)	(37,023,400)	-	-	117,017,400	(43,296,400)	73,721,000	73,721,000	366,474,600
2028	90%	$1.75	315,000,000	-	-	(167,397,500)	(38,504,400)	-	-	109,098,100	(40,366,300)	68,731,800	68,731,800	374,921,400
2029	90%	$1.75	315,000,000	-	30,426,300	(174,093,400)	(40,044,500)	-	-	100,862,100	(37,319,000)	63,543,100	93,969,400	384,963,400

10.2 Economic Sensitivities

To better understand the impact various economic changes will have on expected profits, sensitivity analyses were conducted on the price of acrylic acid, fixed costs, variable costs, and total permanent investment (TPI). To create the spider graph shown in Figure 10.1, each parameter was individually varied between 50% lower than its estimated value and 50% higher than its estimated value. At each new value, the IRR was calculated while holding all other parameters constant.

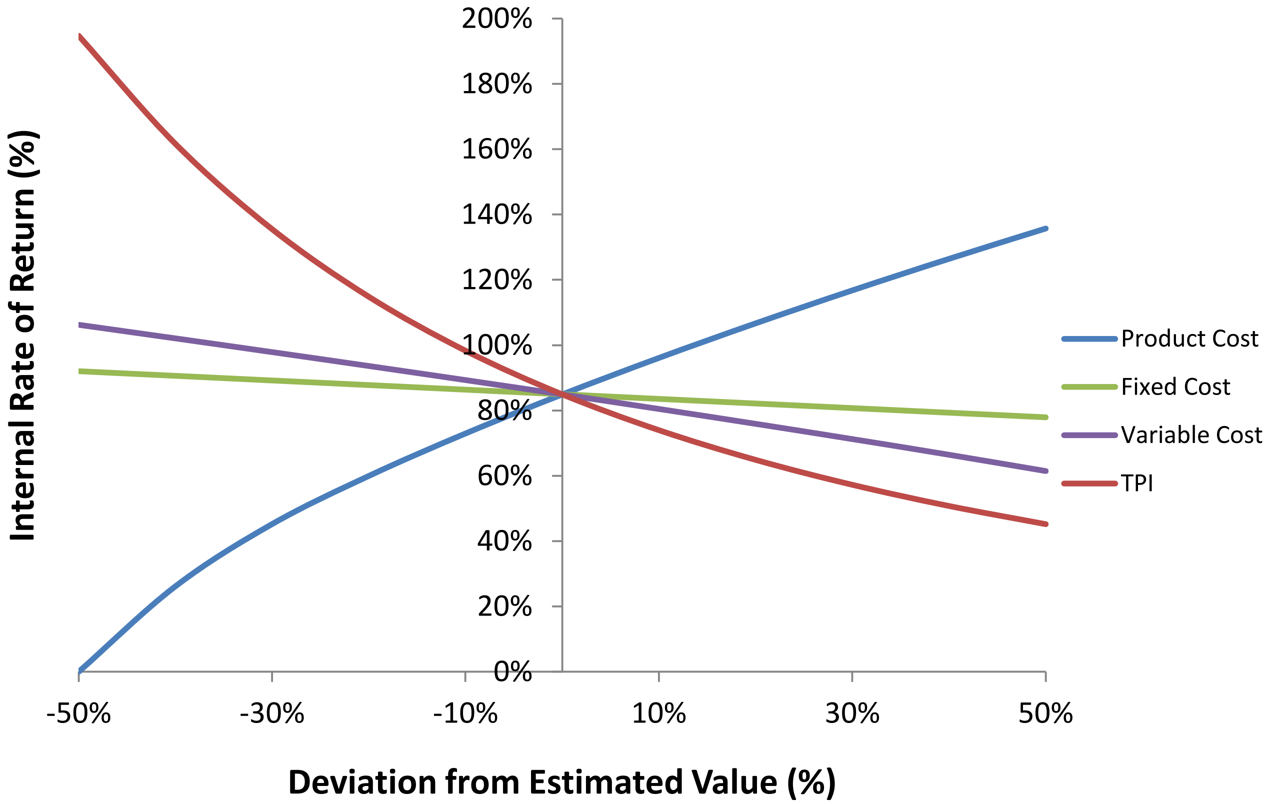

Figure 10.1: Sensitivity Analysis of IRR versus individual parameters

As expected, IRR increases with the increasing price of acrylic acid, and decreases with increasing fixed costs, variable costs, and TPI (Total Permanent Investment). When the price of acrylic acid falls to below 50% of its estimated value the plant is no longer profitable, as evidenced by a negative IRR. This is displayed by the blue curve in Figure 10.1. The TPI most significantly affects the IRR because it is a cost that takes place in the present, and thus will significantly drive the NPV of the project. Even with TPI at 50% higher than its estimated value, the IRR remains above 40%, still suggesting that the project is worth further consideration. It should be noted that the sensitivity analysis does not take into account the relationship between the price and sales of acrylic acid. In a real market, if the price of acrylic acid were to increase to $2.75, sales would likely fall as customers search for alternative products. The actual IRR curve would likely not be as steep as that shown in Figure 10.1, page 114.

Bivariate sensitivity analyses were also conducted to determine which coincident parameters showed the greatest risk for a loss in profitability. In Tables 10.2-4 is evident that if the price of acrylic acid falls to 50% of its estimated value, the fixed costs and/or variable costs would have to fall significantly in order to maintain profitability. This could be a problem in a scenario where the production of acrylic acid from propane becomes extremely widespread. The cost of propane (and thus the variable costs) would rise due to demand and the prices of acrylic acid would fall. Steps must be taken to ensure the process remains profitable by optimizing the process as much as possible and protecting its details as trade secrets in order to maintain a competitive advantage.

Although the expected IRR on the proposed process is approximately 85%, the return is highly sensitive to product price. The quoted selling price of acrylic acid used for the process was $1.75/lb. However, the estimated price for 2012 was listed as $1.20/lb which would bring the IRR down to approximately 45%.[23] The estimated price for 2013 was $1.12-1.16/lb which corresponds to an IRR of 35%.[24] The high volatility in acrylic acid price explains why the return calculated is questionably high. It is suggested that a price of acrylic acid of $1.15/lb would produce a more reasonable estimate of the IRR.

[23] Guzman, D. d. (2012). First 2012 post: OPXBio update. http://www.icis.com/blogs/green-chemicals/2012/01/first-2012-post-opxbio-update.html

[24] Terry, L. (2013). Arkema adds to U.S. March acrylates price-hike efforts.

Table 10.2: Fixed Costs vs. Product Price

Product Price	Fixed Costs										
	$11,562,362	$13,874,835	$16,187,307	$18,499,779	$20,812,252	***$23,124,724***	$25,437,197	$27,749,669	$30,062,142	$32,374,614	$34,687,086
$0.88	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.05	37.15%	35.13%	33.04%	30.87%	28.59%	26.16%	23.53%	20.59%	17.12%	12.48%	Negative IRR
$1.23	53.68%	52.02%	50.35%	48.66%	46.95%	45.23%	43.48%	41.70%	39.89%	38.04%	36.15%
$1.40	67.65%	66.12%	64.59%	63.05%	61.51%	59.96%	58.41%	56.85%	55.28%	53.71%	52.12%
$1.58	80.28%	78.81%	77.35%	75.89%	74.43%	72.97%	71.50%	70.04%	68.57%	67.10%	65.63%
$1.75	91.99%	90.57%	89.15%	87.74%	86.33%	84.92%	83.51%	82.10%	80.69%	79.28%	77.87%
$1.93	103.00%	101.62%	100.24%	98.86%	97.48%	96.11%	94.73%	93.36%	91.99%	90.62%	89.25%
$2.10	113.46%	112.10%	110.75%	109.40%	108.05%	106.70%	105.35%	104.01%	102.67%	101.33%	99.99%
$2.28	123.44%	122.10%	120.77%	119.44%	118.12%	116.79%	115.47%	114.15%	112.83%	111.51%	110.20%
$2.45	133.00%	131.69%	130.38%	129.07%	127.76%	126.46%	125.15%	123.85%	122.55%	121.26%	119.96%
$2.63	142.19%	140.90%	139.61%	138.32%	137.03%	135.74%	134.45%	133.17%	131.89%	130.61%	129.33%

Table 10.3: Variable Costs vs. Product Price

Product Price	Variable Costs										
	$55,852,558	$67,023,069	$78,193,581	$89,364,092	$100,534,604	***$111,705,115***	$122,875,627	$134,046,138	$145,216,650	$156,387,161	$167,557,673
$0.88	43.51%	37.09%	29.76%	20.36%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.05	58.42%	53.04%	47.36%	41.24%	34.41%	26.16%	12.48%	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.23	71.68%	66.80%	61.78%	56.55%	51.07%	45.23%	38.81%	31.37%	21.32%	Negative IRR	Negative IRR
$1.40	83.90%	79.34%	74.69%	69.93%	65.03%	59.96%	54.66%	49.06%	42.99%	36.15%	27.72%
$1.58	95.36%	91.03%	86.63%	82.17%	77.62%	72.97%	68.19%	63.26%	58.13%	52.73%	46.96%
$1.75	106.20%	102.05%	97.85%	93.60%	89.29%	84.92%	80.46%	75.91%	71.25%	66.45%	61.47%
$1.93	116.54%	112.54%	108.49%	104.41%	100.28%	96.11%	91.88%	87.59%	83.22%	78.77%	74.21%
$2.10	126.44%	122.55%	118.64%	114.69%	110.71%	106.70%	102.64%	98.54%	94.39%	90.18%	85.90%
$2.28	135.95%	132.17%	128.36%	124.53%	120.68%	116.79%	112.88%	108.93%	104.94%	100.91%	96.83%
$2.45	145.10%	141.41%	137.70%	133.98%	130.23%	126.46%	122.66%	118.83%	114.98%	111.09%	107.17%
$2.63	153.94%	150.33%	146.71%	143.07%	139.41%	135.74%	132.05%	128.33%	124.59%	120.82%	117.03%

Table 10.4: Total Permanent Investment vs. Product Price

Product Price	Total Permanent Investment										
	$37,937,020	$45,524,424	$53,111,828	$60,699,232	$68,286,636	***$75,874,040***	$83,461,444	$91,048,848	$98,636,252	$106,223,656	$113,811,059
$0.88	33.24%	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
$1.05	82.55%	65.75%	52.57%	42.03%	33.41%	26.16%	19.89%	14.29%	9.07%	3.86%	Negative IRR
$1.23	116.20%	94.49%	77.64%	64.40%	53.83%	45.23%	38.11%	32.14%	27.04%	22.63%	18.77%
$1.40	145.19%	119.12%	98.84%	82.91%	70.22%	59.96%	51.54%	44.53%	38.61%	33.55%	29.18%
$1.58	171.12%	141.29%	117.91%	99.50%	84.82%	72.97%	63.25%	55.18%	48.39%	42.62%	37.65%
$1.75	194.69%	161.61%	135.48%	114.81%	98.28%	84.92%	73.96%	64.87%	57.24%	50.75%	45.19%
$1.93	216.30%	180.43%	151.86%	129.12%	110.89%	96.11%	83.98%	73.91%	65.46%	58.29%	52.14%
$2.10	236.24%	197.98%	167.24%	142.63%	122.81%	106.70%	93.46%	82.46%	73.23%	65.39%	58.67%
$2.28	254.71%	214.42%	181.75%	155.43%	134.14%	116.79%	102.51%	90.62%	80.63%	72.15%	64.88%
$2.45	271.90%	229.87%	195.49%	167.62%	144.97%	126.46%	111.18%	98.45%	87.73%	78.64%	70.84%
$2.63	287.94%	244.43%	208.54%	179.25%	155.35%	135.74%	119.52%	105.98%	94.58%	84.89%	76.58%

Section 11

Conclusions & Recommendations

Though it is traditional to produce acrylic acid from propylene, recent developments in catalyst technology and hydraulic fracturing have made it possible to convert propane to acrylic acid. The objective of this project was to evaluate the feasibility of converting low-cost propane to acrylic acid using the mixed metal oxide catalyst $Mo_1V_{0.30}Te_{0.23}Nb_{0.125}O_x$. It is estimated that such a process producing 200 MM lb/yr acrylic acid will result in an NPV of $384,963,400 over 20 years with an IRR of 84.9% using the assumptions and analysis detailed in this report.

The process will prove profitable even under considerable market fluctuations. The calculated IRR remains positive in virtually all individual sensitivity analyses that were conducted on product price, fixed and variable costs, and TPI. However, in the unlikely event that the price of acrylic acid falls below $0.85/lb, the process can no longer be considered profitable as proposed. In addition, widespread adoption of this process may cause the prices of propane and other variable costs to rise while the prices of acrylic acid fall, which may pose a threat to profitability. Significant technological and design improvements would be required under these scenarios to improve cost efficiency and maintain competitiveness.

An important consideration moving forward with this process is the accuracy of the reactor section design which was based on limited kinetics data. More research is needed to estimate reaction rates and other necessary kinetics parameters. In this analysis, conversion data is based off of patents and published research that was completed with small amounts of catalyst and reactant flow rate. Because this operation is working at such a larger scale, research must be conducted on the effects of scale-up on the catalytic process.

Based on this initial analysis, there are some areas for further investigation. Four pieces of equipment account for 55% of the total equipment cost. These include the recycle stream compressor (C-101), the air compressor (C-102), the Dowtherm pumps (P-103), and the reboiler for the first distillation tower (D-101-REB). Though these pieces of equipment were necessary in the designed process, there may be certain plant configurations that would allow for smaller compressors or reboilers. For example, further considerations for the air compressor might include purchasing compressed nitrogen and mixing it with the pure oxygen stream rather than compressing air in house. Associated costs would be the nitrogen, storage, a turbine for decompression, and a heat exchanger to heat the stream. This might be economically viable if the turbine can produce excess energy that is sent to the grid.

The Dowtherm pump system is a significant cost largely due to the high flow rate and pump head. The cost of pumps is driven by these variables. A different coolant may be examined to reduce the cost of pumps. A coolant with a higher heat capacity (decreasing the needed flow rate) and/or higher density (decreasing the pump head) would decrease the cost of the pump system. However, these changes might increase costs of coolant purchasing price and utility savings currently associated with the Dowtherm heating system.

Our analysis indicates that a propane to acrylic acid process, at current market prices, results in a highly favorable plant system that can make profit by the third year. It is our recommendation that investment in such a process start immediately, to fully capitalize on the current low price of propane by fracking, as well as the current high price of acrylic acid.

Section 12

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Section 13

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Section 14

Appendices

Appendix A: Problem Statement

Suggested Design Projects 2012-2013

6. Propane to Acrylic Acid
(recommended by Bruce M. Vrana, DuPont)

Inexpensive natural gas in the U.S. from fracking is leading to a resurgence in the U.S. chemical industry and a wide array of new possibilities. Propane is now a low cost feedstock in the U.S., because it is produced as part of natural gas liquids from shale oil wells.

Acrylic acid is an important building block in the production of many industrial and consumer products. Most acrylic acid is consumed in polymer form, either directly or after synthesis of an acrylic ester. The esters are in turn consumed as co-monomers, which when polymerized are used in paints, textiles,coatings, adhesives and plastics. Acrylic acid is also polymerized to produce polyacrylic acid-based polymers that are used in superabsorbents, detergent, dispersants, flocculants and thickeners.

Until now, making an unsaturated acid from a saturated hydrocarbon has been elusive (except for butane to maleic anhydride). However, your company has developed a catalyst and one-step process to convert propane to acrylic acid in high yield. The vapor phase catalytic oxidation process has relatively low propane conversion per pass (by feeding an excess of propane compared to oxygen) to keep selectivity high. Propylene is also produced in the process, but can be recycled to the reactor for further reaction, ultimately to acrylic acid.

Your team has been assembled to develop a plant design to put this new catalyst into operation on the U.S. Gulf Coast. Management desires a plant to produce 200MM lb/yr of acrylic acid. They also desire a plant thatuses this technology in the most economical way.

Propane is available by pipeline at your plant site for $0.90/gal. Oxygen can be purchased for $0.03/lb at 500 psig. Acrylic acid can be sold for $1.75/lb. All prices are forecasts by your marketing organization for long-term average prices, expressed in 2013 dollars for the quantities needed delivered to your site or sold from your site.

You will need to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before approving an expensive pilot plant to provide the scale-up data you need to complete the design. Test your economics to reasonable ranges of your assumptions. If there are any possible “show-stoppers” (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

The plant design should be as environmentally friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate.

Remember that, if the plant is approved, you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference

U.S. Patent 8,193,387, June 5, 2012, assigned to Saudi Basic Industries Corp.

Appendix B: Aspen Simulation Input/Report Summary

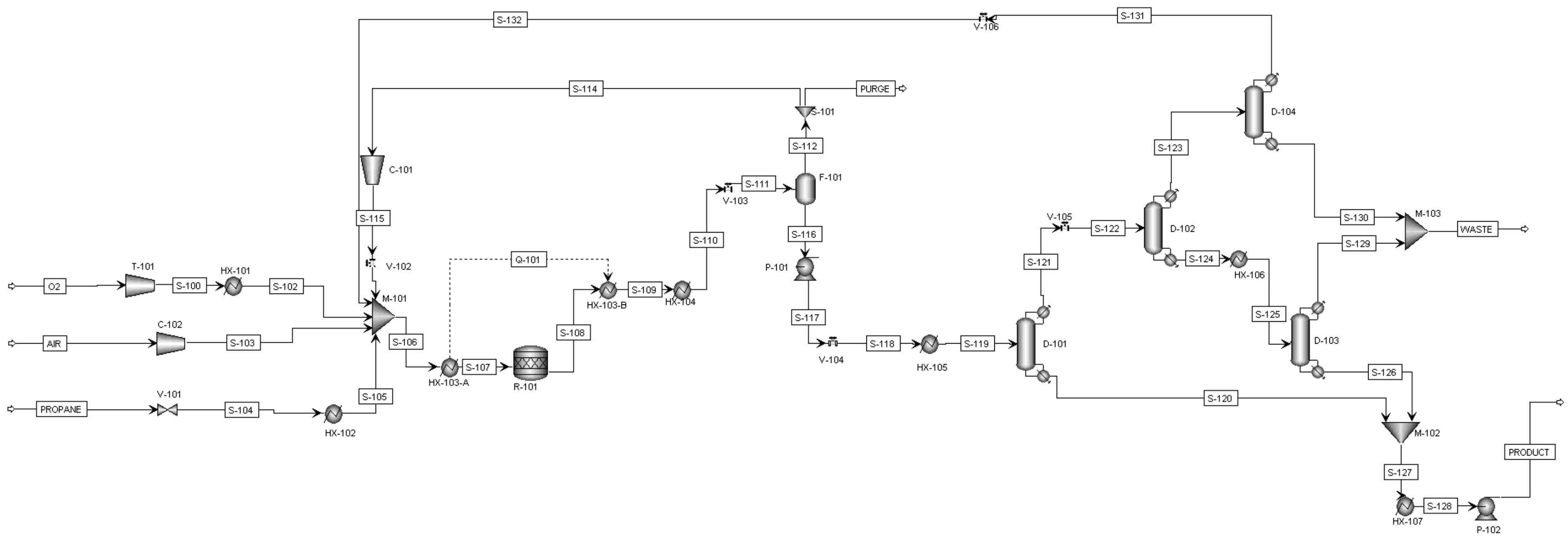

Figure B.1: Overall Aspen Simulation Process

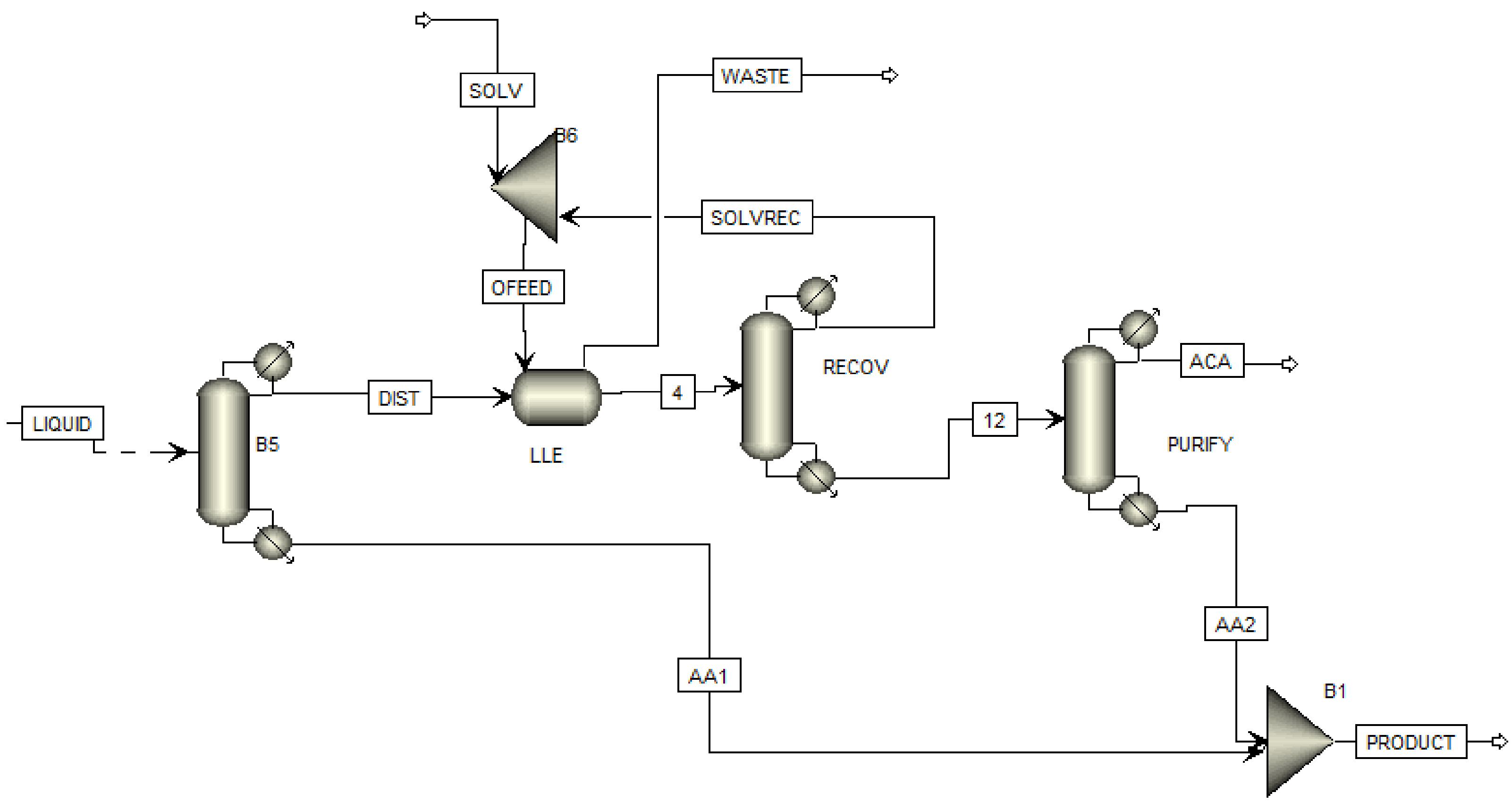

Figure B.2: Preliminary separation process using liquid-liquid extraction techniques

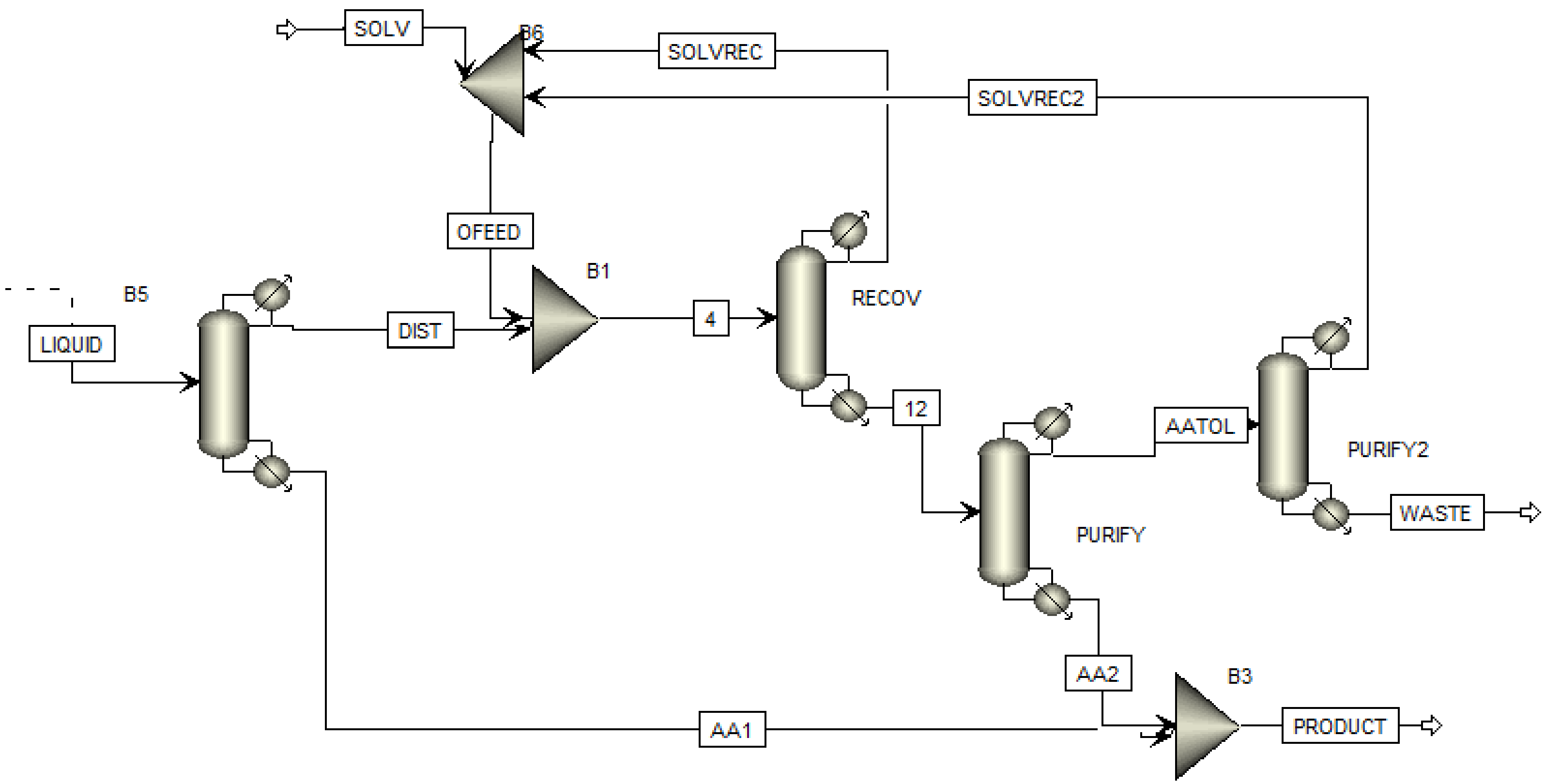

Figure B.3: Preliminary separation processes using extractive distillation techniques

Input Summary

```
DYNAMICS
    DYNAMICS RESULTS=ON

TITLE 'Simple Process'

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

SIM-OPTIONS
    IN-UNITS MET
    SIM-OPTIONS MASS-BAL-CHE=YES TLOWER=9.999989 TUPPER=10000.00  &
        PLOWER=0.0 PUPPER=98692.51 ATM-PRES=1.000000  &
        OLD-DATABANK=YES OPER-YEAR=8766.000 CARBON-FEE=0.0

DATABANKS PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
        NOAspenPCD

PROP-SOURCES PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
    PROPA-01 C3H8 /
    OXYGE-01 O2 /
    PROPY-01 C3H6-2 /
    ACRYL-01 C3H4O2-1 /
    WATER H2O /
    NITROGEN N2 /
    ACETI-01 C2H4O2-1 /
    CARBO-01 CO2 /
    DOWTH-01 DOWA

FLOWSHEET
    BLOCK F-101 IN=S-111 OUT=S-112 S-116
    BLOCK S-101 IN=S-112 OUT=PURGE S-114
    BLOCK R-101 IN=S-107 OUT=S-108
    BLOCK D-102 IN=S-122 OUT=S-123 S-124
    BLOCK D-103 IN=S-125 OUT=S-129 S-126
    BLOCK D-101 IN=S-119 OUT=S-121 S-120
    BLOCK M-102 IN=S-126 S-120 OUT=S-127
    BLOCK D-104 IN=S-123 OUT=S-131 S-130
    BLOCK P-101 IN=S-116 OUT=S-117
    BLOCK HX-105 IN=S-118 OUT=S-119
    BLOCK HX-103-B IN=S-108 Q-101 OUT=S-109
    BLOCK V-103 IN=S-110 OUT=S-111
    BLOCK V-102 IN=S-115 OUT=3
    BLOCK V-104 IN=S-117 OUT=S-118
    BLOCK P-102 IN=S-128 OUT=PRODUCT
    BLOCK V-105 IN=S-121 OUT=S-122
    BLOCK V-106 IN=S-131 OUT=S-132
    BLOCK M-101 IN=S-102 S-103 S-105 3 S-132 OUT=S-106
    BLOCK T-101 IN=O2 OUT=S-100
    BLOCK V-101 IN=PROPANE OUT=S-104
    BLOCK HX-102 IN=S-104 OUT=S-105
    BLOCK HX-101 IN=S-100 OUT=S-102
    BLOCK HX-103-A IN=S-106 OUT=S-107 Q-101
    BLOCK HX-104 IN=S-109 OUT=S-110
    BLOCK C-102 IN=AIR OUT=S-103
    BLOCK HX-106 IN=S-124 OUT=S-125
    BLOCK C-101 IN=S-114 OUT=S-115
```

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    BLOCK HX-107 IN=S-127 OUT=S-128
    BLOCK M-103 IN=S-130 S-129 OUT=WASTE

PROPERTIES NRTL-RK
    PROPERTIES IAPWS-95 / IDEAL / NRTL

PROP-DATA NRTL-1
    IN-UNITS ENG
    PROP-LIST NRTL
    BPVAL ACRYL-01 WATER 0.0 -540.0118757 .3000000000 0.0 0.0  &
        0.0 212.7200023 248.9000020
    BPVAL WATER ACRYL-01 0.0 1663.655567 .3000000000 0.0 0.0  &
        0.0 212.7200023 248.9000020
    BPVAL ACRYL-01 ACETI-01 0.0 76.62239939 .3000000000 0.0  &
        0.0 0.0 244.0400020 284.7200017
    BPVAL ACETI-01 ACRYL-01 0.0 509.4282559 .3000000000 0.0  &
        0.0 0.0 244.0400020 284.7200017
    BPVAL WATER ACETI-01 3.329300000 -1302.998570 .3000000000  &
        0.0 0.0 0.0 68.00000346 445.5500004
    BPVAL ACETI-01 WATER -1.976300000 1097.799471 .3000000000  &
        0.0 0.0 0.0 68.00000346 445.5500004

STREAM AIR
    SUBSTREAM MIXED TEMP=75. PRES=0. <psig> MOLE-FLOW=438.
    MOLE-FRAC OXYGE-01 0.21 / NITROGEN 0.79

STREAM O2
    SUBSTREAM MIXED TEMP=75. PRES=500. MOLE-FLOW=745.
    MASS-FRAC OXYGE-01 1.

STREAM PROPANE
    SUBSTREAM MIXED TEMP=75. PRES=1450. MOLE-FLOW=535.55
    MASS-FRAC PROPA-01 1.

STREAM S-114
    SUBSTREAM MIXED TEMP=85 PRES=25
    MOLE-FLOW PROPA-01 3488.86043 / OXYGE-01 84.7473266 /  &
        PROPY-01 455.074779 / ACRYL-01 24.9502371 / WATER  &
        318.418309 / NITROGEN 11239.0669 / ACETI-01 6.32488207 / &
        CARBO-01 1314.71099

STREAM S-115
    SUBSTREAM MIXED TEMP=225.01242 PRES=59
    MOLE-FLOW PROPA-01 3488.20327 / OXYGE-01 75.7997206 /  &
        PROPY-01 454.993609 / ACRYL-01 24.8537395 / WATER  &
        317.126198 / NITROGEN 11187.9805 / ACETI-01 6.30707424 / &
        CARBO-01 1313.28852

STREAM S-126
    SUBSTREAM MIXED TEMP=389.93742 PRES=69.16
    MOLE-FLOW PROPA-01 1.372612E-015 / PROPY-01 2.966119E-017 /  &
        ACRYL-01 72.3823194 / WATER 0.00038698904 / ACETI-01  &
        0.00031919615 / CARBO-01 1.206147E-023

STREAM S-132
    SUBSTREAM MIXED TEMP=264.178095 PRES=60 MASS-FLOW=5653.26615
    MASS-FRAC PROPA-01 0.498324947 / OXYGE-01 0.00046091140 /  &
        PROPY-01 0.0539472874 / ACRYL-01 0.0195203911 / WATER  &
        0.324403276 / NITROGEN 0.0229753921 / ACETI-01  &
        0.0279930495 / CARBO-01 0.0523747454

DEF-STREAMS HEAT Q-101
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BLOCK M-101 MIXER
    PARAM PRES=54.

BLOCK M-102 MIXER
    PARAM PRES=68. NPHASE=1 PHASE=L MAXIT=100 TOL=0.001
    BLOCK-OPTION FREE-WATER=NO

BLOCK M-103 MIXER
    PARAM PRES=25. MAXIT=100

BLOCK S-101 FSPLIT
    PARAM MAXIT=100 TOL=0.001
    FRAC PURGE 0.03

BLOCK HX-101 HEATER
    PARAM TEMP=230. PRES=-5.

BLOCK HX-102 HEATER
    PARAM TEMP=230. PRES=-5.

BLOCK HX-103-A HEATER
    PARAM TEMP=740. PRES=-5.

BLOCK HX-103-B HEATER
    PARAM PRES=-5.

BLOCK HX-104 HEATER
    PARAM TEMP=85. PRES=-5.

BLOCK HX-105 HEATER
    PARAM TEMP=400. PRES=-5.

BLOCK HX-106 HEATER
    PARAM TEMP=374. PRES=-5.

BLOCK HX-107 HEATER
    PARAM TEMP=100. PRES=-5.

BLOCK F-101 FLASH2
    PARAM TEMP=85. PRES=25.

BLOCK D-101 RADFRAC
    PARAM NSTAGE=13
    COL-CONFIG CONDENSER=PARTIAL-V
    FEEDS S-119 6
    PRODUCTS S-120 13 L / S-121 1 V
    P-SPEC 1 95.
    COL-SPECS D:F=0.764 DP-STAGE=0.12 MOLE-RR=3.5 DP-COND=2.

BLOCK D-102 RADFRAC
    PARAM NSTAGE=14
    COL-CONFIG CONDENSER=PARTIAL-V
    FEEDS S-122 11
    PRODUCTS S-124 14 L / S-123 1 V
    P-SPEC 1 70.
    COL-SPECS D:F=0.8 DP-STAGE=0.12 MOLE-RR=4. DP-COND=2.

BLOCK D-103 RADFRAC
    PARAM NSTAGE=14 MAXOL=100 TOLOL=0.001
    COL-CONFIG CONDENSER=PARTIAL-V
    FEEDS S-125 11
    PRODUCTS S-126 14 L / S-129 1 V
    P-SPEC 1 65.
```

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    COL-SPECS D:F=0.9 DP-STAGE=0.12 MOLE-RR=3. DP-COND=2.

BLOCK D-104 RADFRAC
    PARAM NSTAGE=3
    COL-CONFIG CONDENSER=PARTIAL-V
    FEEDS S-123 2
    PRODUCTS S-130 3 L / S-131 1 V
    P-SPEC 1 65.
    COL-SPECS D:F=0.22 DP-STAGE=0.12 MOLE-RR=4. DP-COND=2.

BLOCK R-101 RSTOIC
    PARAM TEMP=780. PRES=-4. HEAT-OF-REAC=YES
    STOIC 1 MIXED PROPA-01 -1. / OXYGE-01 -0.5 / PROPY-01  &
        1. / WATER 1.
    STOIC 4 MIXED PROPY-01 -1. / OXYGE-01 -1.5 / ACRYL-01  &
        1. / WATER 1.
    STOIC 2 MIXED PROPY-01 -1. / OXYGE-01 -2.5 / ACETI-01  &
        1. / WATER 1. / CARBO-01 1.
    STOIC 3 MIXED ACRYL-01 -1. / OXYGE-01 -3. / CARBO-01 3. / &
        WATER 2.
    STOIC 5 MIXED ACETI-01 -1. / OXYGE-01 -2. / CARBO-01 2. / &
        WATER 2.
    CONV 1 MIXED PROPA-01 0.1
    CONV 4 MIXED PROPY-01 0.8
    CONV 2 MIXED PROPY-01 0.05
    CONV 3 MIXED ACRYL-01 0.001
    CONV 5 MIXED ACETI-01 0.99
    HEAT-RXN REACNO=1 CID=PROPA-01 / REACNO=2 CID=PROPY-01 /  &
        REACNO=3 CID=ACRYL-01 / REACNO=4 CID=PROPY-01 /  &
        REACNO=5 CID=ACETI-01

BLOCK P-101 PUMP
    PARAM PRES=150.

BLOCK P-102 PUMP
    PARAM PRES=75.

BLOCK C-101 COMPR
    PARAM TYPE=ASME-ISENTROP PRES=59. NPHASE=2 MAXIT=100
    BLOCK-OPTION FREE-WATER=NO

BLOCK C-102 COMPR
    PARAM TYPE=ASME-ISENTROP PRES=54.

BLOCK T-101 COMPR
    PARAM TYPE=ISENTROPIC PRES=60. MODEL-TYPE=TURBINE

BLOCK V-101 VALVE
    PARAM P-OUT=60.

BLOCK V-102 VALVE
    PARAM P-DROP=5.

BLOCK V-103 VALVE
    PARAM P-DROP=5.

BLOCK V-104 VALVE
    PARAM P-DROP=20.

BLOCK V-105 VALVE
    PARAM P-DROP=5.

BLOCK V-106 VALVE
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    PARAM P-DROP=5. FLASH-MAXIT=50

STREAM-PRICE
    STREAM-PRICE STREAM=S-127 MASS-PRICE=1.75 / STREAM=PURGE  &
        MASS-PRICE=0. / STREAM=S-130 MASS-PRICE=0. /  &
        STREAM=S-129 MASS-PRICE=0. / STREAM=AIR MASS-PRICE=0. /  &
        STREAM=O2 MASS-PRICE=0.03 / STREAM=PROPANE  &
        MASS-PRICE=0.213

EO-CONV-OPTI
    SM-INIT MAXIT=100 MAXIPASS=100 MAXFITER=100

CONV-OPTIONS
    PARAM TOL=0.001

CONVERGENCE CV-1 WEGSTEIN
    TEAR S-132 1E-005
    PARAM MAXIT=300

CONVERGENCE CV-2 WEGSTEIN
    TEAR S-114 1E-005
    PARAM MAXIT=300

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

REACTIONS R-1 GENERAL
    REAC-DATA 1 NAME=DEHYD PHASE=V
    REAC-DATA 2 NAME=OXID PHASE=V
    RATE-CON 1 PRE-EXP=349465. ACT-ENERGY=62700. <kJ/kmol>
    RATE-CON 2 PRE-EXP=7385. ACT-ENERGY=32900. <kJ/kmol>
    STOIC 1 MIXED PROPA-01 -1. / OXYGE-01 -0.5 / PROPY-01  &
        1. / WATER 1.
    STOIC 2 MIXED PROPY-01 -1. / OXYGE-01 -1.5 / ACRYL-01  &
        1. / WATER 1.
    DFORCE-EXP 1 MIXED PROPA-01 1. / MIXED OXYGE-01 0.
    DFORCE-EXP 2 MIXED PROPY-01 1. / MIXED OXYGE-01 0.23

REACTIONS R-2 GENERAL
    REAC-DATA 1 NAME=DEHYD REAC-CLASS=POWERLAW PHASE=V  &
        PH-BASIS-S=S
    RATE-CON 1 PRE-EXP=349465. ACT-ENERGY=62700. <kJ/kmol>
    STOIC 1 MIXED PROPA-01 -1. / OXYGE-01 -0.5 / PROPY-01  &
        1. / WATER 1.
    DFORCE-EXP 1 MIXED PROPA-01 1. / MIXED OXYGE-01 0.
    REAC-ACT 1
;
;
;
;
;
```

Block Summary

```
BLOCK:  C-101    MODEL: COMPR
-----------------------------
  INLET STREAM:           S-114
  OUTLET STREAM:          S-115
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            16868.6         16868.6         0.00000
      MASS(LB/HR   )            554485.         554485.       -0.419904E-15
      ENTHALPY(BTU/HR  )      -0.411930E+09   -0.388282E+09   -0.574075E-01

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             57797.6      LB/HR
   PRODUCT STREAMS CO2E          57797.6      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  ***

  ISENTROPIC COMPRESSOR USING ASME METHOD
   OUTLET PRESSURE  PSIA                                    59.0000
   ISENTROPIC EFFICIENCY                                     0.72000
   MECHANICAL EFFICIENCY                                     1.00000

                          ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                9,293.95
   BRAKE      HORSEPOWER REQUIREMENT  HP                9,293.95
   NET WORK REQUIRED                  HP                9,293.95
   POWER LOSSES                       HP                    0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                6,691.65
   CALCULATED OUTLET TEMP  F                              225.015
   ISENTROPIC TEMPERATURE  F                              187.599
   EFFICIENCY (POLYTR/ISENTR) USED                          0.72000
   OUTLET VAPOR FRACTION                                    1.00000
   HEAD DEVELOPED,       FT-LBF/LB                     23,895.1
   MECHANICAL EFFICIENCY USED                               1.00000
   INLET HEAT CAPACITY RATIO                                1.26538
   INLET VOLUMETRIC FLOW RATE , CUFT/HR               3,925,990.
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR               2,090,870.
   INLET  COMPRESSIBILITY FACTOR                            0.99546
   OUTLET COMPRESSIBILITY FACTOR                            0.99530
   AV. ISENT. VOL. EXPONENT                                 1.24919
   AV. ISENT. TEMP EXPONENT                                 1.25155
   AV. ACTUAL VOL. EXPONENT                                 1.36287
   AV. ACTUAL TEMP EXPONENT                                 1.36321

BLOCK:  C-102    MODEL: COMPR
-----------------------------
  INLET STREAM:           AIR
  OUTLET STREAM:          S-103
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
```

```
      MOLE(LBMOL/HR)           438.000         438.000         0.00000
      MASS(LB/HR   )           12636.5         12636.5         0.00000
      ENTHALPY(BTU/HR  )      -7396.25        0.100979E+07    -1.00732

                      ***  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  ***

  ISENTROPIC COMPRESSOR USING ASME METHOD
   OUTLET PRESSURE  PSIA                                   54.0000
   ISENTROPIC EFFICIENCY                                    0.72000
   MECHANICAL EFFICIENCY                                    1.00000

                           ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                  399.770
   BRAKE      HORSEPOWER REQUIREMENT  HP                  399.770
   NET WORK REQUIRED                  HP                  399.770
   POWER LOSSES                       HP                    0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                  287.834
   CALCULATED OUTLET TEMP  F                              405.541
   ISENTROPIC TEMPERATURE  F                              313.948
   EFFICIENCY (POLYTR/ISENTR) USED                          0.72000
   OUTLET VAPOR FRACTION                                    1.00000
   HEAD DEVELOPED,       FT-LBF/LB                     45,100.5
   MECHANICAL EFFICIENCY USED                               1.00000
   INLET HEAT CAPACITY RATIO                                1.40086
   INLET VOLUMETRIC FLOW RATE , CUFT/HR               170,928.
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                75,365.0
   INLET  COMPRESSIBILITY FACTOR                            0.99952
   OUTLET COMPRESSIBILITY FACTOR                            1.00072
   AV. ISENT. VOL. EXPONENT                                 1.39779
   AV. ISENT. TEMP EXPONENT                                 1.39639
   AV. ACTUAL VOL. EXPONENT                                 1.58923
   AV. ACTUAL TEMP EXPONENT                                 1.58692

 BLOCK:  D-102    MODEL: RADFRAC
 -------------------------------
   INLETS   - S-122    STAGE  11
   OUTLETS  - S-123    STAGE   1
              S-124    STAGE  14
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                      ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1071.28         1071.28        0.212246E-15
      MASS(LB/HR   )           24750.1         24750.1        0.161687E-14
      ENTHALPY(BTU/HR  )     -0.106050E+09   -0.109605E+09    0.324352E-01

                      ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              308.396      LB/HR
   PRODUCT STREAMS CO2E           308.396      LB/HR
   NET STREAMS CO2E PRODUCTION    0.00000      LB/HR
   UTILITIES CO2E PRODUCTION      0.00000      LB/HR
   TOTAL CO2E PRODUCTION          0.00000      LB/HR
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                    *********************
                    ****  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                    25
  MAXIMUM NO. OF INSIDE LOOP ITERATIONS                     10
  MAXIMUM NUMBER OF FLASH ITERATIONS                        30
  FLASH TOLERANCE                                            0.000100000
  OUTSIDE LOOP CONVERGENCE TOLERANCE                         0.000100000

 ****   COL-SPECS   ****

  MOLAR VAPOR DIST / TOTAL DIST                              1.00000
  MOLAR REFLUX RATIO                                         4.00000
  DISTILLATE TO FEED RATIO                                   0.80000

 ****    PROFILES   ****

  P-SPEC         STAGE   1  PRES, PSIA                      70.0000

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


 ***   COMPONENT SPLIT FRACTIONS   ***

                         OUTLET STREAMS
                         --------------
               S-123        S-124
  COMPONENT:
  PROPA-01    .99999       .14381E-04
  OXYGE-01    1.0000       .11686E-12
  PROPY-01    .99999       .89383E-05
  ACRYL-01    .35817       .64183
  WATER       .79395       .20605
  NITROGEN    1.0000       .29445E-14
  ACETI-01    .93985       .60151E-01
  CARBO-01    1.0000       .17523E-06


 ***    SUMMARY OF KEY RESULTS    ***

  TOP STAGE TEMPERATURE          F                         295.104
  BOTTOM STAGE TEMPERATURE       F                         307.380
  TOP STAGE LIQUID FLOW          LBMOL/HR                3,428.08
  BOTTOM STAGE LIQUID FLOW       LBMOL/HR                  214.255
  TOP STAGE VAPOR FLOW           LBMOL/HR                  857.021
  BOILUP VAPOR FLOW              LBMOL/HR                3,248.61
  MOLAR REFLUX RATIO                                         4.00000
  MOLAR BOILUP RATIO                                        15.1623
  CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                     -0.553158+08
  REBOILER DUTY                  BTU/HR                      0.517608+08
```

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

DEW POINT	0.39186E-08	STAGE= 14	
BUBBLE POINT	0.22660E-06	STAGE= 14	
COMPONENT MASS BALANCE	0.52533E-06	STAGE= 10	COMP=NITROGEN
ENERGY BALANCE	0.38834E-06	STAGE= 14	

**** PROFILES ****

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

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	295.10	70.000	-0.11936E+06	-97192.	-.55316+08
2	302.34	72.000	-0.11997E+06	-0.10202E+06	
9	304.02	72.840	-0.12026E+06	-0.10268E+06	
10	304.17	72.960	-0.12041E+06	-0.10279E+06	
11	305.74	73.080	-0.12070E+06	-0.10418E+06	
12	306.19	73.200	-0.12094E+06	-0.10450E+06	
13	306.58	73.320	-0.12144E+06	-0.10480E+06	
14	307.38	73.440	-0.12280E+06	-0.10542E+06	.51761+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	3428.	857.0					857.0207
2	3426.	4285.					
9	3440.	4293.					
10	3436.	4297.		1071.2759			
11	3437.	3222.					
12	3445.	3223.					
13	3463.	3231.					
14	214.3	3249.				214.2552	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.6967E+05	0.1947E+05					.19472+05
2	0.6859E+05	0.8914E+05					
9	0.7123E+05	0.8995E+05					
10	0.7199E+05	0.9070E+05		.24750+05			
11	0.7243E+05	0.6671E+05					
12	0.7399E+05	0.6716E+05					
13	0.7744E+05	0.6871E+05					
14	5278.	0.7217E+05				5277.8032	

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.15768E-01	0.39670E-06	0.15649E-02	0.21476E-01	0.94437
2	0.52509E-02	0.79426E-07	0.50321E-03	0.23804E-01	0.95680
9	0.38259E-02	0.81199E-07	0.37516E-03	0.40940E-01	0.94607
10	0.38729E-02	0.82046E-07	0.37973E-03	0.45400E-01	0.94148
11	0.72187E-03	0.37832E-09	0.64511E-04	0.50539E-01	0.94136
12	0.13693E-03	0.17737E-11	0.11155E-04	0.59233E-01	0.93450
13	0.26813E-04	0.85947E-14	0.19922E-05	0.76391E-01	0.91836
14	0.55570E-05	0.44441E-16	0.37691E-06	0.11880	0.87651

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.10701E-04	0.16260E-01	0.54909E-03
2	0.21390E-05	0.13495E-01	0.14237E-03
9	0.22055E-05	0.86633E-02	0.12431E-03
10	0.22288E-05	0.87360E-02	0.12577E-03
11	0.49221E-08	0.73020E-02	0.98549E-05
12	0.11058E-10	0.61166E-02	0.78693E-06
13	0.25683E-13	0.52197E-02	0.65038E-07
14	0.63719E-16	0.46813E-02	0.57311E-08

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.96601E-01	0.95071E-04	0.10542E-01	0.16574E-01	0.84432
2	0.31935E-01	0.19332E-04	0.33603E-02	0.20495E-01	0.92436
9	0.22316E-01	0.19044E-04	0.24018E-02	0.33245E-01	0.92861
10	0.22328E-01	0.19025E-04	0.24027E-02	0.36081E-01	0.92578
11	0.41301E-02	0.87502E-07	0.40496E-03	0.40519E-01	0.94580
12	0.76949E-03	0.40347E-09	0.68775E-04	0.46001E-01	0.94567
13	0.14564E-03	0.18913E-11	0.11870E-04	0.55283E-01	0.93835
14	0.28214E-04	0.91586E-14	0.20987E-05	0.73593E-01	0.92112

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.54101E-02	0.18286E-01	0.81765E-02
2	0.10906E-02	0.16665E-01	0.20746E-02
9	0.10818E-02	0.10595E-01	0.17309E-02
10	0.10807E-02	0.10582E-01	0.17301E-02
11	0.23770E-05	0.90056E-02	0.13413E-03
12	0.52493E-08	0.74763E-02	0.10510E-04
13	0.11791E-10	0.62118E-02	0.83874E-06
14	0.27373E-13	0.52552E-02	0.68950E-07

**** K-VALUES ****

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	6.1264	239.65	6.7365	0.77176	0.89405
2	6.0817	243.39	6.6777	0.86100	0.96609
9	5.8330	234.54	6.4021	0.81203	0.98155
10	5.7650	231.88	6.3272	0.79474	0.98332
11	5.7214	231.29	6.2774	0.80174	1.0047
12	5.6197	227.47	6.1651	0.77660	1.0120
13	5.4318	220.06	5.9584	0.72369	1.0218
14	5.0773	206.08	5.5683	0.61947	1.0509

**** K-VALUES ****

STAGE	NITROGEN	ACETI-01	CARBO-01
1	505.56	1.1246	14.891
2	509.86	1.2349	14.572
9	490.51	1.2229	13.924
10	484.88	1.2113	13.756
11	482.92	1.2333	13.611
12	474.73	1.2223	13.355
13	459.08	1.1901	12.896
14	429.59	1.1226	12.031

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.34214E-01	0.62462E-06	0.32403E-02	0.76152E-01	0.83714
2	0.11565E-01	0.12694E-06	0.10576E-02	0.85677E-01	0.86091
9	0.81485E-02	0.12549E-06	0.76250E-03	0.14250	0.82320
10	0.81520E-02	0.12532E-06	0.76275E-03	0.15617	0.80961
11	0.15105E-02	0.57442E-09	0.12881E-03	0.17282	0.80472

```
   12    0.28113E-03   0.26426E-11   0.21857E-04   0.19874       0.78385
   13    0.52868E-04   0.12297E-13   0.37485E-05   0.24615       0.73978
   14    0.99476E-05   0.57729E-16   0.64387E-06   0.34755       0.64103

                      ****   MASS-X-PROFILE     ****
  STAGE     NITROGEN      ACETI-01      CARBO-01
    1    0.14751E-04   0.48047E-01   0.11891E-02
    2    0.29927E-05   0.40477E-01   0.31293E-03
    9    0.29840E-05   0.25128E-01   0.26423E-03
   10    0.29802E-05   0.25042E-01   0.26421E-03
   11    0.65428E-08   0.20808E-01   0.20580E-04
   12    0.14422E-10   0.17102E-01   0.16125E-05
   13    0.32171E-13   0.14016E-01   0.12799E-06
   14    0.72463E-16   0.11412E-01   0.10239E-07

                      ****   MASS-Y-PROFILE     ****
  STAGE     PROPA-01      OXYGE-01      PROPY-01      ACRYL-01      WATER
    1    0.18748       0.13389E-03   0.19524E-01   0.52568E-01   0.66945
    2    0.67694E-01   0.29736E-04   0.67974E-02   0.71000E-01   0.80051
    9    0.46965E-01   0.29083E-04   0.48236E-02   0.11434       0.79840
   10    0.46648E-01   0.28843E-04   0.47903E-02   0.12319       0.79019
   11    0.87962E-02   0.13523E-06   0.82305E-03   0.14103       0.82295
   12    0.16284E-02   0.61957E-09   0.13889E-03   0.15908       0.81758
   13    0.30196E-03   0.28456E-11   0.23486E-04   0.18731       0.79482
   14    0.56006E-04   0.13192E-13   0.39756E-05   0.23874       0.74700

                      ****   MASS-Y-PROFILE     ****
  STAGE     NITROGEN      ACETI-01      CARBO-01
    1    0.66703E-02   0.48332E-01   0.15838E-01
    2    0.14686E-02   0.48109E-01   0.43890E-02
    9    0.14463E-02   0.30364E-01   0.36355E-02
   10    0.14343E-02   0.30109E-01   0.36076E-02
   11    0.32160E-05   0.26120E-01   0.28511E-03
   12    0.70570E-08   0.21546E-01   0.22197E-04
   13    0.15530E-10   0.17539E-01   0.17356E-05
   14    0.34519E-13   0.14206E-01   0.13660E-06

 BLOCK:  D-103    MODEL: RADFRAC
 -------------------------------
   INLETS   - S-125    STAGE  11
   OUTLETS  - S-129    STAGE   1
              S-126    STAGE  14
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          214.255          214.255          0.00000
      MASS(LB/HR   )          5277.80          5277.80       -0.367070E-10
      ENTHALPY(BTU/HR  )    -0.227940E+08   -0.231893E+08    0.170470E-01

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.540407E-04  LB/HR
   PRODUCT STREAMS CO2E         0.540407E-04  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  ****
                      **********************
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****   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                                  30
 FLASH TOLERANCE                                                      0.000100000
 OUTSIDE LOOP CONVERGENCE TOLERANCE                                   0.00100000

****   COL-SPECS   ****

 MOLAR VAPOR DIST / TOTAL DIST                                        1.00000
 MOLAR REFLUX RATIO                                                   3.00000
 DISTILLATE TO FEED RATIO                                             0.90000

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIA                               65.0000

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


***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
              S-129         S-126
 COMPONENT:
 PROPA-01    1.0000        .48570E-05
 PROPY-01    1.0000        .30864E-05
 ACRYL-01    .21351        .78649
 WATER       .99260        .73979E-02
 ACETI-01    .98297        .17033E-01
 CARBO-01    1.0000        .72527E-07


***    SUMMARY OF KEY RESULTS    ***

 TOP STAGE TEMPERATURE          F                                  298.050
 BOTTOM STAGE TEMPERATURE       F                                  371.435
 TOP STAGE LIQUID FLOW          LBMOL/HR                           578.489
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                            21.4255
 TOP STAGE VAPOR FLOW           LBMOL/HR                           192.830
 BOILUP VAPOR FLOW              LBMOL/HR                           659.513
 MOLAR REFLUX RATIO                                                  3.00000
 MOLAR BOILUP RATIO                                                 30.7816
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                      -9,425,590.
 REBOILER DUTY                  BTU/HR                       9,030,480.

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

 DEW POINT                        0.53295E-03  STAGE=  8
 BUBBLE POINT                     0.10798E-02  STAGE= 12
 COMPONENT MASS BALANCE           0.14232E-05  STAGE=  7 COMP=PROPA-01
```

ENERGY BALANCE 0.22651E-02 STAGE= 14

**** PROFILES ****

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

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	298.05	65.000	-0.12006E+06	-0.10375E+06	-.94256+07
2	300.11	67.000	-0.12009E+06	-0.10376E+06	
9	301.58	67.840	-0.12186E+06	-0.10487E+06	
10	302.29	67.960	-0.12304E+06	-0.10539E+06	
11	303.66	68.080	-0.12518E+06	-0.10613E+06	
12	310.96	68.200	-0.13273E+06	-0.10862E+06	
13	339.57	68.320	-0.14351E+06	-0.11714E+06	
14	371.43	68.440	-0.14858E+06	-0.12962E+06	.90305+07

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	578.5	192.8					192.8296
2	580.5	771.3					
9	591.4	780.7					
10	588.0	784.3		214.2552			
11	597.7	566.6					
12	624.3	576.2					
13	680.9	602.9					
14	21.43	659.5				21.4255	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1151E+05	3809.					3809.0983
2	0.1165E+05	0.1532E+05					
9	0.1364E+05	0.1679E+05					
10	0.1469E+05	0.1745E+05		5277.8032			
11	0.1702E+05	0.1322E+05					
12	0.2541E+05	0.1555E+05					
13	0.4017E+05	0.2394E+05					
14	1469.	0.3870E+05				1468.7049	

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

STAGE	PROPA-01	PROPY-01	ACRYL-01	WATER	ACETI-01
1	0.94199E-06	0.58115E-07	0.31811E-01	0.96429	0.38957E-02
2	0.35367E-06	0.21211E-07	0.35390E-01	0.96139	0.32222E-02
9	0.31315E-06	0.19084E-07	0.91357E-01	0.90587	0.27735E-02
10	0.33034E-06	0.20125E-07	0.12655	0.87047	0.29870E-02
11	0.68599E-07	0.38069E-08	0.19119	0.80592	0.28919E-02
12	0.13995E-07	0.70864E-09	0.41758	0.57966	0.27690E-02
13	0.21441E-08	0.99730E-10	0.75673	0.24147	0.18023E-02
14	0.26990E-09	0.11633E-10	0.93436	0.64843E-01	0.79738E-03

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

STAGE	CARBO-01
1	0.40074E-09
2	0.12331E-09
9	0.12368E-09

10	0.13023E-09
11	0.11307E-10
12	0.97955E-12
13	0.67854E-13
14	0.41566E-14

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

STAGE	PROPA-01	PROPY-01	ACRYL-01	WATER	ACETI-01
1	0.61744E-05	0.41878E-06	0.28184E-01	0.96670	0.51129E-02
2	0.22501E-05	0.14828E-06	0.30904E-01	0.96489	0.42000E-02
9	0.17526E-05	0.11731E-06	0.62061E-01	0.93468	0.32578E-02
10	0.17543E-05	0.11736E-06	0.75824E-01	0.92082	0.33487E-02
11	0.34282E-06	0.20885E-07	0.95998E-01	0.90093	0.30698E-02
12	0.71139E-07	0.39480E-08	0.16355	0.83348	0.29698E-02
13	0.14483E-07	0.73341E-09	0.39921	0.59795	0.28390E-02
14	0.22049E-08	0.10259E-09	0.75096	0.24721	0.18349E-02

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

STAGE	CARBO-01
1	0.63679E-08
2	0.18925E-08
9	0.16629E-08
10	0.16590E-08
11	0.13516E-09
12	0.11727E-10
13	0.10142E-11
14	0.69923E-13

**** K-VALUES ****

STAGE	PROPA-01	PROPY-01	ACRYL-01	WATER	ACETI-01
1	6.5522	7.2034	0.88536	1.0025	1.3120
2	6.3590	6.9874	0.87242	1.0037	1.3029
9	5.6026	6.1536	0.67980	1.0312	1.1749
10	5.3150	5.8368	0.60022	1.0574	1.1219
11	5.0072	5.4969	0.50338	1.1172	1.0626
12	5.0863	5.5748	0.39265	1.4353	1.0730
13	6.7692	7.3703	0.52762	2.4752	1.5758
14	8.1832	8.8345	0.80374	3.8129	2.3020

**** K-VALUES ****

STAGE	CARBO-01
1	15.885
2	15.341
9	13.464
10	12.752
11	11.976
12	11.980
13	14.991
14	16.826

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

STAGE	PROPA-01	PROPY-01	ACRYL-01	WATER	ACETI-01
1	0.20875E-05	0.12290E-06	0.11521	0.87303	0.11757E-01
2	0.77732E-06	0.44488E-07	0.12711	0.86324	0.96444E-02
9	0.59858E-06	0.34811E-07	0.28538	0.70740	0.72197E-02
10	0.58313E-06	0.33901E-07	0.36506	0.62776	0.71807E-02
11	0.10625E-06	0.56269E-08	0.48393	0.50997	0.60999E-02
12	0.15162E-07	0.73266E-09	0.73934	0.25657	0.40855E-02
13	0.16027E-08	0.71142E-10	0.92442	0.73743E-01	0.18347E-02
14	0.17362E-09	0.71411E-11	0.98226	0.17041E-01	0.69855E-03

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

STAGE CARBO-01

```
     1    0.88633E-09
     2    0.27047E-09
     9    0.23594E-09
    10    0.22944E-09
    11    0.17479E-10
    12    0.10592E-11
    13    0.50622E-13
    14    0.26686E-14

                        ****   MASS-Y-PROFILE     ****
  STAGE     PROPA-01      PROPY-01      ACRYL-01      WATER         ACETI-01
     1    0.13783E-04   0.89212E-06   0.10282       0.88162       0.15544E-01
     2    0.49955E-05   0.31416E-06   0.11213       0.87517       0.12698E-01
     9    0.35934E-05   0.22953E-06   0.20795       0.78295       0.90968E-02
    10    0.34761E-05   0.22192E-06   0.24553       0.74543       0.90364E-02
    11    0.64790E-06   0.37666E-07   0.29649       0.69561       0.79009E-02
    12    0.11627E-06   0.61577E-08   0.43685       0.55654       0.66102E-02
    13    0.16082E-07   0.77717E-09   0.72444       0.27127       0.42933E-02
    14    0.16569E-08   0.73571E-10   0.92223       0.75895E-01   0.18778E-02

                        ****   MASS-Y-PROFILE     ****
  STAGE     CARBO-01
     1    0.14187E-07
     2    0.41934E-08
     9    0.34028E-08
    10    0.32808E-08
    11    0.25493E-09
    12    0.19130E-10
    13    0.11240E-11
    14    0.52442E-13

 BLOCK:  D-101    MODEL: RADFRAC
 -------------------------------
   INLETS   - S-119    STAGE   6
   OUTLETS  - S-121    STAGE   1
              S-120    STAGE  13
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1402.19          1402.19         0.00000
      MASS(LB/HR   )            48595.6          48595.6        0.161852E-12
      ENTHALPY(BTU/HR  )      -0.150858E+09   -0.155488E+09    0.297751E-01

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              308.396      LB/HR
   PRODUCT STREAMS CO2E           308.396      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  ****
                        *********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                        13
   ALGORITHM OPTION                                      STANDARD
   ABSORBER OPTION                                       NO
```

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

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	1.00000
MOLAR REFLUX RATIO	3.50000
DISTILLATE TO FEED RATIO	0.76400

**** PROFILES ****

P-SPEC	STAGE 1	PRES, PSIA	95.0000

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	S-121	S-120
COMPONENT:		
PROPA-01	1.0000	.26702E-07
OXYGE-01	1.0000	0.0000
PROPY-01	1.0000	.14026E-07
ACRYL-01	.10703	.89297
WATER	.99997	.25794E-04
NITROGEN	1.0000	0.0000
ACETI-01	.99853	.14700E-02
CARBO-01	1.0000	.55131E-11

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	318.087
BOTTOM STAGE TEMPERATURE	F	418.132
TOP STAGE LIQUID FLOW	LBMOL/HR	3,749.47
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	330.918
TOP STAGE VAPOR FLOW	LBMOL/HR	1,071.28
BOILUP VAPOR FLOW	LBMOL/HR	4,592.06
MOLAR REFLUX RATIO		3.50000
MOLAR BOILUP RATIO		13.8767
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.586925+08
REBOILER DUTY	BTU/HR	0.540628+08

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

DEW POINT	0.18399E-06	STAGE= 7	
BUBBLE POINT	0.81478E-06	STAGE= 6	
COMPONENT MASS BALANCE	0.17057E-05	STAGE= 5	COMP=NITROGEN
ENERGY BALANCE	0.34872E-06	STAGE= 6	

**** PROFILES ****

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

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	318.09	95.000	-0.11968E+06	-98994.	-.58692+08
2	323.69	97.000	-0.12080E+06	-0.10291E+06	
4	325.68	97.240	-0.12308E+06	-0.10453E+06	
5	328.44	97.360	-0.12682E+06	-0.10584E+06	
6	336.53	97.480	-0.13315E+06	-0.10934E+06	
11	417.49	98.080	-0.14939E+06	-0.13749E+06	
12	417.94	98.200	-0.14940E+06	-0.13760E+06	
13	418.13	98.320	-0.14940E+06	-0.13763E+06	.54063+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	3749.	1071.					1071.2759
2	3760.	4821.					
4	3830.	4854.					
5	3852.	4901.		1402.1936			
6	3972.	3521.					
11	4918.	4568.					
12	4923.	4587.					
13	330.9	4592.				330.9177	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.8227E+05	0.2475E+05					.24750+05
2	0.8428E+05	0.1070E+06					
4	0.9948E+05	0.1140E+06					
5	0.1234E+06	0.1242E+06		.48596+05			
6	0.1655E+06	0.9957E+05					
11	0.3541E+06	0.3278E+06					
12	0.3547E+06	0.3302E+06					
13	0.2385E+05	0.3308E+06				.23846+05	

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.16653E-01	0.39612E-06	0.16628E-02	0.52310E-01	0.91429
2	0.67251E-02	0.91323E-07	0.64775E-03	0.67585E-01	0.91174
4	0.51811E-02	0.97917E-07	0.50745E-03	0.13468	0.84680
5	0.54855E-02	0.10273E-06	0.53822E-03	0.24591	0.73423
6	0.15110E-02	0.64911E-09	0.13626E-03	0.42549	0.55827
11	0.25760E-06	0.29297E-21	0.16664E-07	0.99828	0.12666E-02
12	0.41661E-07	0.87175E-24	0.25363E-08	0.99951	0.30194E-03
13	0.66803E-08	0.25937E-26	0.38294E-09	0.99985	0.71043E-04

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.10924E-04	0.14458E-01	0.61358E-03
2	0.25087E-05	0.13105E-01	0.18991E-03
4	0.27141E-05	0.12652E-01	0.17082E-03
5	0.28548E-05	0.13650E-01	0.18248E-03
6	0.88984E-08	0.14563E-01	0.22806E-04
11	0.15775E-21	0.45405E-03	0.36257E-10
12	0.24973E-24	0.18510E-03	0.20619E-11

13	0.39542E-27	0.74179E-04	0.11674E-12

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.77282E-01	0.76057E-04	0.84335E-02	0.37020E-01	0.85075
2	0.30126E-01	0.17210E-04	0.31674E-02	0.48912E-01	0.90017
4	0.21097E-01	0.16857E-04	0.22542E-02	0.78677E-01	0.88228
5	0.20942E-01	0.16702E-04	0.22400E-02	0.11333	0.84767
6	0.60011E-02	0.11239E-06	0.58881E-03	0.17505	0.80323
11	0.17043E-05	0.10542E-18	0.11719E-06	0.99317	0.56556E-02
12	0.27570E-06	0.31411E-21	0.17838E-07	0.99817	0.13529E-02
13	0.44181E-07	0.93438E-24	0.26914E-08	0.99949	0.31858E-03

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.43281E-02	0.15565E-01	0.65412E-02
2	0.97029E-03	0.14704E-01	0.19308E-02
4	0.95711E-03	0.13150E-01	0.15710E-02
5	0.94820E-03	0.13289E-01	0.15633E-02
6	0.31232E-05	0.14926E-01	0.19963E-03
11	0.10673E-18	0.11771E-02	0.68100E-09
12	0.16913E-21	0.48145E-03	0.38864E-10
13	0.26769E-24	0.19309E-03	0.22021E-11

**** K-VALUES ****

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	4.6407	192.01	5.0720	0.70769	0.93051
2	4.4797	188.45	4.8898	0.72372	0.98731
4	4.0718	172.15	4.4422	0.58417	1.0419
5	3.8176	162.58	4.1619	0.46087	1.1545
6	3.9715	173.14	4.3212	0.41140	1.4388
11	6.6162	359.83	7.0327	0.99488	4.4650
12	6.6179	360.32	7.0334	0.99865	4.4807
13	6.6136	360.25	7.0284	0.99963	4.4843

**** K-VALUES ****

STAGE	NITROGEN	ACETI-01	CARBO-01
1	396.19	1.0766	10.661
2	386.76	1.1221	10.167
4	352.64	1.0394	9.1971
5	332.14	0.97349	8.5671
6	350.98	1.0249	8.7537
11	676.60	2.5924	18.783
12	677.24	2.6011	18.849
13	676.99	2.6030	18.862

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.33469E-01	0.57771E-06	0.31890E-02	0.17181	0.75071
2	0.13230E-01	0.13037E-06	0.12161E-02	0.21728	0.73278
4	0.87946E-02	0.12061E-06	0.82199E-03	0.37361	0.58724
5	0.75495E-02	0.10260E-06	0.70687E-03	0.55308	0.41283
6	0.15991E-02	0.49848E-09	0.13761E-03	0.73588	0.24137
11	0.15779E-06	0.13022E-21	0.97407E-08	0.99930	0.31698E-03
12	0.25499E-07	0.38719E-24	0.14814E-08	0.99977	0.75501E-04
13	0.40880E-08	0.11518E-26	0.22363E-09	0.99992	0.17761E-04

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.13948E-04	0.39573E-01	0.12307E-02
2	0.31353E-05	0.35109E-01	0.37287E-03
4	0.29268E-05	0.29246E-01	0.28938E-03
5	0.24960E-05	0.25584E-01	0.25065E-03

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    6    0.59824E-08   0.20989E-01   0.24087E-04
   11    0.61384E-22   0.37876E-03   0.22165E-10
   12    0.97102E-25   0.15429E-03   0.12596E-11
   13    0.15372E-27   0.61820E-04   0.71302E-13

                      ****   MASS-Y-PROFILE     ****
  STAGE     PROPA-01      OXYGE-01      PROPY-01      ACRYL-01      WATER
    1    0.14750       0.10534E-03   0.15361E-01   0.11547       0.66339
    2    0.59843E-01   0.24807E-04   0.60041E-02   0.15878       0.73052
    4    0.39628E-01   0.22977E-04   0.40408E-02   0.24152       0.67706
    5    0.36429E-01   0.21083E-04   0.37184E-02   0.32218       0.60241
    6    0.93576E-02   0.12717E-06   0.87616E-03   0.44606       0.51169
   11    0.10476E-05   0.47020E-19   0.68738E-07   0.99759       0.14202E-02
   12    0.16889E-06   0.13963E-21   0.10428E-07   0.99926       0.33858E-03
   13    0.27042E-07   0.41501E-24   0.15721E-08   0.99976       0.79663E-04

                      ****   MASS-Y-PROFILE     ****
  STAGE     NITROGEN      ACETI-01      CARBO-01
    1    0.52479E-02   0.40459E-01   0.12460E-01
    2    0.12244E-02   0.39778E-01   0.38279E-02
    4    0.11421E-02   0.33638E-01   0.29452E-02
    5    0.10478E-02   0.31480E-01   0.27141E-02
    6    0.30938E-05   0.31697E-01   0.31068E-03
   11    0.41675E-19   0.98528E-03   0.41775E-09
   12    0.65817E-22   0.40165E-03   0.23761E-10
   13    0.10409E-24   0.16095E-03   0.13452E-11

 BLOCK:  D-104    MODEL: RADFRAC
 -------------------------------
    INLETS   - S-123    STAGE   2
    OUTLETS  - S-131    STAGE   1
               S-130    STAGE   3
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN                OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            857.021          857.021          0.00000
       MASS(LB/HR   )            19472.3          19472.3        -0.192035E-10
       ENTHALPY(BTU/HR  )      -0.832956E+08   -0.941029E+08    0.114846

                    ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             308.396      LB/HR
    PRODUCT STREAMS CO2E          308.396      LB/HR
    NET STREAMS CO2E PRODUCTION  0.623277E-07  LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION        0.623277E-07  LB/HR


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

   ****   INPUT PARAMETERS   ****

    NUMBER OF STAGES                                           3
    ALGORITHM OPTION                                        STANDARD
    ABSORBER OPTION                                         NO
    INITIALIZATION OPTION                                   STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                        NO
    INSIDE LOOP CONVERGENCE METHOD                          BROYDEN
    DESIGN SPECIFICATION METHOD                             NESTED
```

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

****   COL-SPECS   ****

 MOLAR VAPOR DIST / TOTAL DIST                            1.00000
 MOLAR REFLUX RATIO                                       4.00000
 DISTILLATE TO FEED RATIO                                 0.22000

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIA                   65.0000

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


***   COMPONENT SPLIT FRACTIONS   ***

                          OUTLET STREAMS
                          --------------
              S-131        S-130
 COMPONENT:
 PROPA-01    .77167       .22833
 OXYGE-01    .99998       .22899E-04
 PROPY-01    .80219       .19781
 ACRYL-01    .10781       .89219
 WATER       .14068       .85932
 NITROGEN   1.0000        .23489E-05
 ACETI-01    .16815       .83185
 CARBO-01    .96009       .39914E-01


***    SUMMARY OF KEY RESULTS    ***

 TOP STAGE TEMPERATURE          F                       264.767
 BOTTOM STAGE TEMPERATURE       F                       286.858
 TOP STAGE LIQUID FLOW          LBMOL/HR                754.178
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                668.476
 TOP STAGE VAPOR FLOW           LBMOL/HR                188.545
 BOILUP VAPOR FLOW              LBMOL/HR                 88.8219
 MOLAR REFLUX RATIO                                       4.00000
 MOLAR BOILUP RATIO                                       0.13287
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                  -0.121879+08
 REBOILER DUTY                  BTU/HR           1,380,580.

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

 DEW POINT                        0.26868E-08  STAGE=  2
 BUBBLE POINT                     0.11769E-07  STAGE=  2
 COMPONENT MASS BALANCE           0.38566E-06  STAGE=  2 COMP=NITROGEN
 ENERGY BALANCE                   0.54171E-07  STAGE=  1


****    PROFILES   ****

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

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	264.77	65.000	-0.11660E+06	-78574.	-.12188+08
2	277.18	67.000	-0.11730E+06	-84809.	
3	286.86	67.120	-0.11861E+06	-91936.	.13806+07

STAGE	FLOW RATE LBMOL/HR LIQUID	FLOW RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR LIQUID	FEED RATE LBMOL/HR VAPOR	FEED RATE LBMOL/HR MIXED	PRODUCT RATE LBMOL/HR LIQUID	PRODUCT RATE LBMOL/HR VAPOR
1	754.2	188.5		857.0207			188.5445
2	757.3	85.70					
3	668.5	88.82				668.4762	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR LIQUID	FLOW RATE LB/HR VAPOR	FEED RATE LB/HR LIQUID	FEED RATE LB/HR VAPOR	FEED RATE LB/HR MIXED	PRODUCT RATE LB/HR LIQUID	PRODUCT RATE LB/HR VAPOR
1	0.1619E+05	5653.		.19472+05			5653.2420
2	0.1602E+05	2372.					
3	0.1382E+05	2199.				.13819+05	

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.56529E-01	0.20394E-05	0.58016E-02	0.17965E-01	0.89812
2	0.45619E-01	0.80158E-07	0.45109E-02	0.18258E-01	0.91094
3	0.28278E-01	0.27911E-08	0.26735E-02	0.18958E-01	0.93017

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.53405E-04	0.19206E-01	0.23183E-02
2	0.97874E-06	0.19544E-01	0.11243E-02
3	0.16292E-07	0.19502E-01	0.41840E-03

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.33884	0.43213E-03	0.38439E-01	0.81219E-02	0.53992
2	0.27689	0.17925E-04	0.30201E-01	0.10217E-01	0.64817
3	0.17613	0.66243E-06	0.18339E-01	0.12991E-01	0.76623

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

STAGE	NITROGEN	ACETI-01	CARBO-01
1	0.24591E-01	0.13977E-01	0.35683E-01
2	0.46983E-03	0.16900E-01	0.17138E-01
3	0.82222E-05	0.19860E-01	0.64366E-02

**** K-VALUES ****

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	5.9940	211.89	6.6255	0.45210	0.60116
2	6.0695	223.62	6.6952	0.55957	0.71154
3	6.2286	237.33	6.8598	0.68525	0.82376

**** K-VALUES ****

STAGE	NITROGEN	ACETI-01	CARBO-01
1	460.47	0.72772	15.391
2	480.04	0.86475	15.244
3	504.69	1.0184	15.384

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

STAGE	PROPA-01	OXYGE-01	PROPY-01	ACRYL-01	WATER
1	0.11611	0.30397E-05	0.11372E-01	0.60303E-01	0.75366

```
     2    0.95108E-01   0.12127E-06   0.89745E-02   0.62207E-01   0.77588
     3    0.60320E-01   0.43204E-08   0.54421E-02   0.66088E-01   0.81061

                        ****   MASS-X-PROFILE     ****
   STAGE     NITROGEN      ACETI-01      CARBO-01
     1    0.69686E-04   0.53725E-01   0.47525E-02
     2    0.12963E-05   0.55489E-01   0.23393E-02
     3    0.22077E-07   0.56652E-01   0.89074E-03

                        ****   MASS-Y-PROFILE     ****
   STAGE     PROPA-01      OXYGE-01      PROPY-01      ACRYL-01      WATER
     1    0.49832       0.46118E-03   0.53947E-01   0.19520E-01   0.32440
     2    0.44116       0.20724E-04   0.45919E-01   0.26602E-01   0.42190
     3    0.31375       0.85627E-06   0.31175E-01   0.37819E-01   0.55763

                        ****   MASS-Y-PROFILE     ****
   STAGE     NITROGEN      ACETI-01      CARBO-01
     1    0.22975E-01   0.27993E-01   0.52375E-01
     2    0.47555E-03   0.36670E-01   0.27252E-01
     3    0.93046E-05   0.48180E-01   0.11443E-01

 BLOCK:  F-101    MODEL: FLASH2
 ------------------------------
   INLET STREAM:           S-111
   OUTLET VAPOR STREAM:    S-112
   OUTLET LIQUID STREAM:   S-116
   PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           18792.5         18792.5        0.193587E-15
       MASS(LB/HR   )           620230.         620230.         0.00000
       ENTHALPY(BTU/HR  )      -0.605822E+09   -0.603439E+09   -0.393374E-02

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             59893.6      LB/HR
    PRODUCT STREAMS CO2E          59893.6      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   TP  FLASH
   SPECIFIED TEMPERATURE F                                   85.0000
   SPECIFIED PRESSURE    PSIA                                25.0000
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE                                      0.000100000

                          ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     85.000
   OUTLET PRESSURE       PSIA                                  25.000
   HEAT DUTY             BTU/HR                               0.23831E+07
   VAPOR FRACTION                                             0.92539


   V-L PHASE EQUILIBRIUM :

      COMP             F(I)           X(I)           Y(I)           K(I)
      PROPA-01       0.19576       0.59043E-01    0.20679         3.5023
      OXYGE-01       0.41650E-02   0.58108E-04    0.44961E-02     77.375
      PROPY-01       0.25441E-01   0.64432E-02    0.26973E-01     4.1862
```

```
     ACRYL-01         0.21080E-01    0.26425        0.14734E-02    0.55757E-02
     WATER            0.65896E-01    0.64999        0.18800E-01    0.28923E-01
     NITROGEN         0.61400        0.33066E-02    0.66324         200.58
     ACETI-01         0.12346E-02    0.11909E-01    0.37389E-03    0.31395E-01
     CARBO-01         0.72418E-01    0.49975E-02    0.77854E-01     15.579

 BLOCK:  HX-101   MODEL: HEATER
 ------------------------------
   INLET STREAM:          S-100
   OUTLET STREAM:         S-102
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN                OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           745.000          745.000          0.00000
       MASS(LB/HR   )           23839.1          23839.1          0.00000
       ENTHALPY(BTU/HR  )       -975531.         800285.         -1.82036

                    ***  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  TP  FLASH
   SPECIFIED TEMPERATURE              F                        230.000
   PRESSURE DROP                      PSI                        5.00000
   MAXIMUM NO. ITERATIONS                                       30
   CONVERGENCE TOLERANCE                                         0.000100000



                         ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                   230.00
   OUTLET PRESSURE       PSIA                                55.000
   HEAT DUTY             BTU/HR                             0.17758E+07
   OUTLET VAPOR FRACTION                                     1.0000
   PRESSURE-DROP CORRELATION PARAMETER                       19906.



   V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     OXYGE-01          1.0000         1.0000         1.0000         210.52

 BLOCK:  HX-102   MODEL: HEATER
 ------------------------------
   INLET STREAM:          S-104
   OUTLET STREAM:         S-105
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN                OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           535.550          535.550          0.00000
       MASS(LB/HR   )           23615.9          23615.9          0.00000
       ENTHALPY(BTU/HR  )     -0.277925E+08   -0.225617E+08   -0.188208

                    ***  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  TP  FLASH
SPECIFIED TEMPERATURE              F                        230.000
PRESSURE DROP                      PSI                        5.00000
MAXIMUM NO. ITERATIONS                                       30
CONVERGENCE TOLERANCE                                         0.000100000



                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                   230.00
OUTLET PRESSURE       PSIA                                55.000
HEAT DUTY             BTU/HR                             0.52308E+07
OUTLET VAPOR FRACTION                                     1.0000
PRESSURE-DROP CORRELATION PARAMETER                       37231.



V-L PHASE EQUILIBRIUM :

   COMP             F(I)          X(I)          Y(I)          K(I)
   PROPA-01         1.0000        1.0000        1.0000        6.6568

BLOCK:  HX-105   MODEL: HEATER
------------------------------
  INLET STREAM:          S-118
  OUTLET STREAM:         S-119
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
 TOTAL BALANCE
    MOLE(LBMOL/HR)            1402.19         1402.19         0.00000
    MASS(LB/HR   )            48595.6         48595.6         0.00000
    ENTHALPY(BTU/HR  )      -0.178734E+09   -0.150858E+09   -0.155965

                    ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E            308.396      LB/HR
 PRODUCT STREAMS CO2E         308.396      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  TP  FLASH
SPECIFIED TEMPERATURE              F                        400.000
PRESSURE DROP                      PSI                        5.00000
MAXIMUM NO. ITERATIONS                                       30
CONVERGENCE TOLERANCE                                         0.000100000



                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                   400.00
OUTLET PRESSURE       PSIA                                125.00
HEAT DUTY             BTU/HR                             0.27876E+08
OUTLET VAPOR FRACTION                                     1.0000
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  PRESSURE-DROP CORRELATION PARAMETER                        14410.


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     PROPA-01         0.59043E-01    0.21586E-01    0.59043E-01     4.1359
     OXYGE-01         0.58108E-04    0.40821E-06    0.58108E-04     215.24
     PROPY-01         0.64432E-02    0.22035E-02    0.64432E-02     4.4214
     ACRYL-01         0.26425        0.58345        0.26425        0.68484
     WATER            0.64999        0.38053        0.64999         2.5828
     NITROGEN         0.33066E-02    0.12152E-04    0.33066E-02     411.46
     ACETI-01         0.11909E-01    0.11483E-01    0.11909E-01     1.5682
     CARBO-01         0.49975E-02    0.73161E-03    0.49975E-02     10.329

BLOCK:  HX-104   MODEL: HEATER
------------------------------
  INLET STREAM:           S-109
  OUTLET STREAM:          S-110
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           18792.5         18792.5         0.00000
      MASS(LB/HR   )           620230.         620230.         0.00000
      ENTHALPY(BTU/HR  )      -0.542769E+09   -0.605822E+09    0.104079

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            59893.6      LB/HR
   PRODUCT STREAMS CO2E         59893.6      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  TP  FLASH
  SPECIFIED TEMPERATURE               F                        85.0000
  PRESSURE DROP                       PSI                       5.00000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   85.000
  OUTLET PRESSURE       PSIA                                35.000
  HEAT DUTY             BTU/HR                            -0.63054E+08
  OUTLET VAPOR FRACTION                                     0.91694
  PRESSURE-DROP CORRELATION PARAMETER                       17.050


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     PROPA-01         0.19576        0.78640E-01    0.20637         2.6243
     OXYGE-01         0.41650E-02    0.78769E-04    0.45351E-02     57.574
     PROPY-01         0.25441E-01    0.86023E-02    0.26966E-01     3.1347
     ACRYL-01         0.21080E-01    0.24273        0.10030E-02    0.41322E-02
     WATER            0.65896E-01    0.64682        0.13276E-01    0.20526E-01
     NITROGEN         0.61400        0.44834E-02    0.66921         149.27
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```
    ACETI-01         0.12346E-02    0.11899E-01    0.26862E-03    0.22574E-01
    CARBO-01         0.72418E-01    0.67411E-02    0.78367E-01     11.625

BLOCK:  HX-103-B MODEL: HEATER
------------------------------
   INLET STREAM:           S-108
   INLET HEAT STREAM:      Q-101
   OUTLET STREAM:          S-109
   PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT         RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           18792.5         18792.5         0.00000
       MASS(LB/HR   )           620230.         620230.         0.00000
       ENTHALPY(BTU/HR  )      -0.542769E+09   -0.542769E+09     0.00000

                    ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E              59893.6      LB/HR
    PRODUCT STREAMS CO2E           59893.6      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  PQ  FLASH
   PRESSURE DROP                        PSI                         5.00000
   DUTY FROM INLET HEAT STREAM(S)       BTU/HR                     -0.118784+09
   MAXIMUM NO. ITERATIONS                                          30
   CONVERGENCE TOLERANCE                                            0.000100000



                         ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     280.13
   OUTLET PRESSURE       PSIA                                  40.000
   OUTLET VAPOR FRACTION                                       1.0000
   PRESSURE-DROP CORRELATION PARAMETER                         12.095



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      PROPA-01         0.19576        0.37052E-01    0.19576         9.4119
      OXYGE-01         0.41650E-02    0.31539E-04    0.41650E-02     363.06
      PROPY-01         0.25441E-01    0.42317E-02    0.25441E-01     10.407
      ACRYL-01         0.21080E-01    0.61978        0.21080E-01    0.36140
      WATER            0.65896E-01    0.32507        0.65896E-01     1.5500
      NITROGEN         0.61400        0.19565E-02    0.61400         777.28
      ACETI-01         0.12346E-02    0.70964E-02    0.12346E-02     1.0553
      CARBO-01         0.72418E-01    0.47873E-02    0.72418E-01     24.043

BLOCK:  HX-103-A MODEL: HEATER
------------------------------
   INLET STREAM:           S-106
   OUTLET STREAM:          S-107
   OUTLET HEAT STREAM:     Q-101
   PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT         RELATIVE DIFF.
    TOTAL BALANCE
```

```
      MOLE(LBMOL/HR)           18775.7         18775.7          0.00000
      MASS(LB/HR   )           620230.         620230.          0.00000
      ENTHALPY(BTU/HR  )     -0.423848E+09   -0.423848E+09      0.00000

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             58093.7      LB/HR
   PRODUCT STREAMS CO2E          58093.7      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  TP  FLASH
  SPECIFIED TEMPERATURE              F                         740.000
  PRESSURE DROP                      PSI                         5.00000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    740.00
  OUTLET PRESSURE       PSIA                                 49.000
  HEAT DUTY             BTU/HR                              0.11878E+09
  OUTLET VAPOR FRACTION                                      1.0000
  PRESSURE-DROP CORRELATION PARAMETER                        14.975



  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     PROPA-01         0.21771        0.76158        0.21771        46.058
     OXYGE-01         0.48622E-01    0.32936E-02    0.48622E-01    2378.5
     PROPY-01         0.24619E-01    0.68765E-01    0.24619E-01    57.683
     ACRYL-01         0.14053E-02    0.18518E-01    0.14053E-02    12.228
     WATER            0.22312E-01    0.93129E-01    0.22312E-01    38.607
     NITROGEN         0.61455        0.28202E-01    0.61455        3510.9
     ACETI-01         0.47627E-03    0.55514E-02    0.47627E-03    13.824
     CARBO-01         0.70305E-01    0.20961E-01    0.70305E-01    540.41

 BLOCK:  HX-106   MODEL: HEATER
 ------------------------------
  INLET STREAM:          S-124
  OUTLET STREAM:         S-125
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           214.255         214.255          0.00000
      MASS(LB/HR   )           5277.80         5277.80        0.344649E-15
      ENTHALPY(BTU/HR  )     -0.263095E+08   -0.227940E+08   -0.133619

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.540407E-04  LB/HR
   PRODUCT STREAMS CO2E        0.540407E-04  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  TP  FLASH
```

```
  SPECIFIED TEMPERATURE                F                       374.000
  PRESSURE DROP                        PSI                       5.00000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    374.00
  OUTLET PRESSURE       PSIA                                 68.440
  HEAT DUTY             BTU/HR                             0.35154E+07
  OUTLET VAPOR FRACTION                                      1.0000
  PRESSURE-DROP CORRELATION PARAMETER                      0.47984E+06



  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     PROPA-01         0.55570E-05    0.21989E-05    0.55570E-05     6.1544
     PROPY-01         0.37691E-06    0.13802E-06    0.37691E-06     6.6502
     ACRYL-01         0.11880        0.23831        0.11880         1.2140
     WATER            0.87651        0.75669        0.87651         2.8210
     ACETI-01         0.46813E-02    0.49992E-02    0.46813E-02     2.2804
     CARBO-01         0.57311E-08    0.10730E-08    0.57311E-08     13.007

BLOCK:  HX-107   MODEL: HEATER
------------------------------
  INLET STREAM:           S-127
  OUTLET STREAM:          S-128
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            352.343         352.343         0.00000
      MASS(LB/HR   )            25314.2         25314.2         0.00000
      ENTHALPY(BTU/HR  )      -0.526212E+08   -0.550982E+08    0.449552E-01

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.170415E-08  LB/HR
   PRODUCT STREAMS CO2E         0.170415E-08  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  TP  FLASH
  SPECIFIED TEMPERATURE                F                       100.000
  PRESSURE DROP                        PSI                       5.00000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    100.00
  OUTLET PRESSURE       PSIA                                 63.000
  HEAT DUTY             BTU/HR                            -0.24769E+07
  OUTLET VAPOR FRACTION                                      0.0000
  PRESSURE-DROP CORRELATION PARAMETER                      0.30597E+07
```

```
  V-L PHASE EQUILIBRIUM :

     COMP              F(I)            X(I)            Y(I)            K(I)
     PROPA-01        0.62905E-08     0.62905E-08     0.43465E-05      2.4471
     PROPY-01        0.36036E-09     0.36036E-09     0.29142E-06      2.8641
     ACRYL-01        0.99587         0.99587         0.97717         0.34751E-02
     WATER           0.40097E-02     0.40097E-02     0.21960E-01     0.19396E-01
     ACETI-01        0.11816E-03     0.11816E-03     0.86428E-03     0.25906E-01
     CARBO-01        0.10990E-12     0.10990E-12     0.26821E-09      8.6436

 BLOCK:  M-101    MODEL: MIXER
 -----------------------------
   INLET STREAMS:         S-102       S-103       S-105       3           S-132
   OUTLET STREAM:         S-106
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          18775.7         18775.7         0.00000
       MASS(LB/HR   )          620230.         620230.        0.375394E-15
       ENTHALPY(BTU/HR  )    -0.423848E+09   -0.423848E+09   -0.562509E-15

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             58093.7      LB/HR
    PRODUCT STREAMS CO2E          58093.7      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      FLASH
   MAXIMUM NO. ITERATIONS                                 30
   CONVERGENCE TOLERANCE                                   0.000100000
   OUTLET PRESSURE   PSIA                                54.0000

 BLOCK:  M-102    MODEL: MIXER
 -----------------------------
   INLET STREAMS:         S-126       S-120
   OUTLET STREAM:         S-127
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          352.343         352.343         0.00000
       MASS(LB/HR   )          25314.2         25314.2         0.00000
       ENTHALPY(BTU/HR  )    -0.526212E+08   -0.526212E+08   -0.283178E-15

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E           0.170415E-08  LB/HR
    PRODUCT STREAMS CO2E        0.170415E-08  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  ***
   ONE    PHASE      FLASH   SPECIFIED PHASE IS  LIQUID
   MAXIMUM NO. ITERATIONS                                100
   CONVERGENCE TOLERANCE                                   0.00100000
   OUTLET PRESSURE   PSIA                                68.0000
```

```
BLOCK:  M-103    MODEL: MIXER
-----------------------------
  INLET STREAMS:          S-130       S-129
  OUTLET STREAM:          WASTE
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           861.306         861.306         0.00000
      MASS(LB/HR   )           17628.2         17628.2       -0.412746E-15
      ENTHALPY(BTU/HR  )     -0.992941E+08   -0.992941E+08    0.450213E-15

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            12.3093      LB/HR
   PRODUCT STREAMS CO2E         12.3093      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     FLASH
  MAXIMUM NO. ITERATIONS                                   100
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE   PSIA                                   25.0000

BLOCK:  P-101    MODEL: PUMP
----------------------------
  INLET STREAM:           S-116
  OUTLET STREAM:          S-117
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1402.19         1402.19         0.00000
      MASS(LB/HR   )           48595.6         48595.6       -0.149724E-15
      ENTHALPY(BTU/HR  )     -0.178770E+09   -0.178734E+09   -0.196145E-03

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            308.396      LB/HR
   PRODUCT STREAMS CO2E         308.396      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                                  150.000
   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                          814.794
   PRESSURE CHANGE  PSI                                   125.000
   NPSH AVAILABLE   FT-LBF/LB                               0.0
   FLUID POWER  HP                                          7.40722
   BRAKE POWER  HP                                         13.7810
   ELECTRICITY  KW                                         10.2765
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    PUMP EFFICIENCY USED                                       0.53749
    NET WORK REQUIRED  HP                                      13.7810
    HEAD DEVELOPED FT-LBF/LB                                   301.803

 BLOCK:  R-101    MODEL: RSTOIC
 ------------------------------
   INLET STREAM:          S-107
   OUTLET STREAM:         S-108
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                            IN          OUT       GENERATION   RELATIVE DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         18775.7       18792.5       16.8089     -0.193587E-15
   MASS(LB/HR   )         620230.       620230.                     0.00000
   ENTHALPY(BTU/HR  )   -0.305064E+09 -0.423985E+09                 0.280483

                     ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             58093.7      LB/HR
    PRODUCT STREAMS CO2E          59893.6      LB/HR
    NET STREAMS CO2E PRODUCTION   1799.86      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
    TOTAL CO2E PRODUCTION         1799.86      LB/HR

                         ***  INPUT DATA  ***
   STOICHIOMETRY MATRIX:

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

    REACTION #   2:
     SUBSTREAM MIXED   :
     OXYGE-01  -2.50    PROPY-01  -1.00    WATER      1.00    ACETI-01   1.00
     CARBO-01   1.00

    REACTION #   3:
     SUBSTREAM MIXED   :
     OXYGE-01  -3.00    ACRYL-01  -1.00    WATER      2.00    CARBO-01   3.00

    REACTION #   4:
     SUBSTREAM MIXED   :
     OXYGE-01  -1.50    PROPY-01  -1.00    ACRYL-01   1.00    WATER      1.00

    REACTION #   5:
     SUBSTREAM MIXED   :
     OXYGE-01  -2.00    WATER      2.00    ACETI-01  -1.00    CARBO-01   2.00


   REACTION CONVERSION SPECS: NUMBER=    5
     REACTION #   1:
     SUBSTREAM:MIXED    KEY COMP:PROPA-01 CONV FRAC: 0.1000
     REACTION #   2:
     SUBSTREAM:MIXED    KEY COMP:PROPY-01 CONV FRAC: 0.5000E-01
     REACTION #   3:
     SUBSTREAM:MIXED    KEY COMP:ACRYL-01 CONV FRAC: 0.1000E-02
     REACTION #   4:
     SUBSTREAM:MIXED    KEY COMP:PROPY-01 CONV FRAC: 0.8000
     REACTION #   5:
     SUBSTREAM:MIXED    KEY COMP:ACETI-01 CONV FRAC: 0.9900
```

```
TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                 780.000
PRESSURE DROP         PSI                                 4.00000
MAXIMUM NO. ITERATIONS                                   30
CONVERGENCE TOLERANCE                                     0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                   780.00
OUTLET PRESSURE       PSIA                                45.000
HEAT DUTY             BTU/HR                            -0.11892E+09
VAPOR FRACTION                                            1.0000



HEAT OF REACTIONS:

  REACTION          REFERENCE          HEAT OF
  NUMBER            COMPONENT          REACTION
                                        BTU/LBMOL
   1                   PROPA-01          -50297.
   2                   PROPY-01        -0.46801E+06
   3                   ACRYL-01        -0.57059E+06
   4                   PROPY-01        -0.25768E+06
   5                   ACETI-01        -0.36024E+06

REACTION EXTENTS:

   REACTION          REACTION
   NUMBER            EXTENT
                     LBMOL/HR
   1                  408.76
   2                  23.112
   3                 0.26385E-01
   4                  369.79
   5                  8.8529

V-L PHASE EQUILIBRIUM :

   COMP              F(I)           X(I)           Y(I)           K(I)
   PROPA-01         0.19576        0.48479        0.19576        62.657
   OXYGE-01         0.41650E-02    0.23325E-03    0.41650E-02    2770.7
   PROPY-01         0.25441E-01    0.49883E-01    0.25441E-01    79.136
   ACRYL-01         0.21080E-01    0.21460        0.21080E-01    15.239
   WATER            0.65896E-01    0.20087        0.65896E-01    50.900
   NITROGEN         0.61400        0.23870E-01    0.61400        3991.3
   ACETI-01         0.12346E-02    0.10802E-01    0.12346E-02    17.733
   CARBO-01         0.72418E-01    0.14952E-01    0.72418E-01    751.51

BLOCK:  S-101    MODEL: FSPLIT
------------------------------
  INLET STREAM:          S-112
  OUTLET STREAMS:        PURGE       S-114
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          17390.3          17390.3         0.473668E-07
      MASS(LB/HR   )          571634.          571634.         0.645727E-07
      ENTHALPY(BTU/HR  )    -0.424670E+09   -0.424670E+09     0.313680E-06
```

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                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            59585.2      LB/HR
   PRODUCT STREAMS CO2E         59585.2      LB/HR
   NET STREAMS CO2E PRODUCTION  0.511356E-03  LB/HR
   UTILITIES CO2E PRODUCTION     0.00000     LB/HR
   TOTAL CO2E PRODUCTION        0.511356E-03  LB/HR

                      ***  INPUT DATA  ***

 FRACTION OF FLOW                 STRM=PURGE    FRAC=         0.030000

                       ***  RESULTS  ***

 STREAM= PURGE          SPLIT=          0.030000    KEY=  0    STREAM-ORDER=   1
         S-114                          0.97000           0                    2

BLOCK:  P-102    MODEL: PUMP
----------------------------
  INLET STREAM:          S-128
  OUTLET STREAM:         PRODUCT
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          352.343         352.343         0.00000
      MASS(LB/HR   )          25314.2         25314.2         0.00000
      ENTHALPY(BTU/HR  )    -0.550982E+08   -0.550962E+08   -0.362655E-04

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.170415E-08  LB/HR
   PRODUCT STREAMS CO2E        0.170415E-08  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                                     75.0000
   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                            393.107
   PRESSURE CHANGE  PSI                                      12.0000
   NPSH AVAILABLE   FT-LBF/LB                               140.467
   FLUID POWER  HP                                            0.34307
   BRAKE POWER  HP                                            0.78531
   ELECTRICITY  KW                                            0.58560
   PUMP EFFICIENCY USED                                       0.43687
   NET WORK REQUIRED  HP                                      0.78531
   HEAD DEVELOPED FT-LBF/LB                                  26.8342

BLOCK:  T-101    MODEL: COMPR
-----------------------------
  INLET STREAM:          O2
  OUTLET STREAM:         S-100
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
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```
                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT         RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          745.000         745.000         0.00000
       MASS(LB/HR   )          23839.1         23839.1         0.00000
       ENTHALPY(BTU/HR  )     -97842.6        -975531.        0.899703

                  ***  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  ***

   ISENTROPIC TURBINE
    OUTLET PRESSURE  PSIA                                      60.0000
    ISENTROPIC EFFICIENCY                                       0.72000
    MECHANICAL EFFICIENCY                                       1.00000

                       ***  RESULTS  ***

    INDICATED  HORSEPOWER REQUIREMENT  HP                    -344.945
    BRAKE      HORSEPOWER REQUIREMENT  HP                    -344.945
    NET WORK REQUIRED                  HP                    -344.945
    POWER LOSSES                       HP                       0.0
    ISENTROPIC HORSEPOWER REQUIREMENT  HP                    -479.090
    CALCULATED OUTLET TEMP  F                                -106.462
    ISENTROPIC TEMPERATURE  F                                -170.573
    EFFICIENCY (POLYTR/ISENTR) USED                             0.72000
    OUTLET VAPOR FRACTION                                       1.00000
    HEAD DEVELOPED,       FT-LBF/LB                       -39,791.7
    MECHANICAL EFFICIENCY USED                                  1.00000
    INLET HEAT CAPACITY RATIO                                   1.45910
    INLET VOLUMETRIC FLOW RATE , CUFT/HR                    8,343.26
    OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                   46,416.5
    INLET  COMPRESSIBILITY FACTOR                               0.97590
    OUTLET COMPRESSIBILITY FACTOR                               0.98624
    AV. ISENT. VOL. EXPONENT                                    1.40972
    AV. ISENT. TEMP EXPONENT                                    1.40846
    AV. ACTUAL VOL. EXPONENT                                    1.23544
    AV. ACTUAL TEMP EXPONENT                                    1.24307

  BLOCK:  V-102    MODEL: VALVE
  -----------------------------
   INLET STREAM:          S-115
   OUTLET STREAM:         3
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT         RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          16868.6         16868.6         0.00000
       MASS(LB/HR   )          554485.         554485.         0.00000
       ENTHALPY(BTU/HR  )    -0.388282E+09   -0.388282E+09     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             57797.6      LB/HR
    PRODUCT STREAMS CO2E          57797.6      LB/HR
    NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
    UTILITIES CO2E PRODUCTION     0.00000      LB/HR
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   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                      ***  INPUT DATA  ***

   VALVE PRESSURE DROP       PSI                           5.00000
   VALVE FLOW COEF CALC.                                 NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                  2
   MAX NUMBER OF ITERATIONS                               30
   CONVERGENCE TOLERANCE                                   0.000100000

                      ***  RESULTS  ***

   VALVE OUTLET PRESSURE     PSIA                         54.0000

 BLOCK:  V-103    MODEL: VALVE
 -----------------------------
   INLET STREAM:          S-110
   OUTLET STREAM:         S-111
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           18792.5         18792.5         0.00000
      MASS(LB/HR   )           620230.         620230.         0.00000
      ENTHALPY(BTU/HR  )     -0.605822E+09   -0.605822E+09     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             59893.6      LB/HR
   PRODUCT STREAMS CO2E          59893.6      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  ***

   VALVE PRESSURE DROP       PSI                           5.00000
   VALVE FLOW COEF CALC.                                 NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                  2
   MAX NUMBER OF ITERATIONS                               30
   CONVERGENCE TOLERANCE                                   0.000100000

                      ***  RESULTS  ***

   VALVE OUTLET PRESSURE     PSIA                         30.0000

 BLOCK:  V-101    MODEL: VALVE
 -----------------------------
   INLET STREAM:          PROPANE
   OUTLET STREAM:         S-104
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           535.550         535.550         0.00000
      MASS(LB/HR   )           23615.9         23615.9         0.00000
      ENTHALPY(BTU/HR  )     -0.277925E+08   -0.277925E+08     0.00000
```

```
                  ***  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  ***

   VALVE OUTLET PRESSURE     PSIA                          60.0000
   VALVE FLOW COEF CALC.                                  NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                   2
   MAX NUMBER OF ITERATIONS                                30
   CONVERGENCE TOLERANCE                                    0.000100000

                      ***  RESULTS  ***

   VALVE PRESSURE DROP       PSI                         1,390.00

 BLOCK:  V-104    MODEL: VALVE
 -----------------------------
   INLET STREAM:          S-117
   OUTLET STREAM:         S-118
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1402.19         1402.19         0.00000
      MASS(LB/HR   )           48595.6         48595.6         0.00000
      ENTHALPY(BTU/HR  )     -0.178734E+09   -0.178734E+09     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              308.396      LB/HR
   PRODUCT STREAMS CO2E           308.396      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  ***

   VALVE PRESSURE DROP       PSI                           20.0000
   VALVE FLOW COEF CALC.                                  NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                   2
   MAX NUMBER OF ITERATIONS                                30
   CONVERGENCE TOLERANCE                                    0.000100000

                      ***  RESULTS  ***

   VALVE OUTLET PRESSURE     PSIA                         130.000

 BLOCK:  V-105    MODEL: VALVE
 -----------------------------
   INLET STREAM:          S-121
   OUTLET STREAM:         S-122
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
```

```
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1071.28         1071.28         0.00000
      MASS(LB/HR   )            24750.1         24750.1         0.00000
      ENTHALPY(BTU/HR  )      -0.106050E+09   -0.106050E+09     0.00000

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             308.396      LB/HR
   PRODUCT STREAMS CO2E          308.396      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  ***

   VALVE PRESSURE DROP       PSI                              5.00000
   VALVE FLOW COEF CALC.                                    NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                     2
   MAX NUMBER OF ITERATIONS                                  30
   CONVERGENCE TOLERANCE                                      0.000100000

                      ***  RESULTS  ***

   VALVE OUTLET PRESSURE     PSIA                            90.0000

BLOCK:  V-106    MODEL: VALVE
-----------------------------
  INLET STREAM:            S-131
  OUTLET STREAM:           S-132
  PROPERTY OPTION SET:     NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            188.545         188.545       -0.136709E-07
      MASS(LB/HR   )            5653.24         5653.24        0.603530E-07
      ENTHALPY(BTU/HR  )      -0.148147E+08   -0.148147E+08    0.216899E-07

                  ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             296.087      LB/HR
   PRODUCT STREAMS CO2E          296.087      LB/HR
   NET STREAMS CO2E PRODUCTION -0.583838E-06  LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION       -0.583838E-06  LB/HR

                      ***  INPUT DATA  ***

   VALVE PRESSURE DROP       PSI                              5.00000
   VALVE FLOW COEF CALC.                                    NO

                      FLASH SPECIFICATIONS:
   NPHASE                                                     2
   MAX NUMBER OF ITERATIONS                                  50
   CONVERGENCE TOLERANCE                                      0.000100000

                      ***  RESULTS  ***

   VALVE OUTLET PRESSURE     PSIA                            60.0000
```

Appendix C: Design Calculations

Mole Balance across Reactor

Carbon balance:

$$Carbon\ in = \sum (flowrate)\left(\frac{1}{MW}\right)\left(\frac{mol\ Carbon}{mol\ species}\right)$$

$$= \left(180250\ \frac{lb}{hr}\ propane\right)\left(\frac{1\ lbmol}{44.1\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ propane}\right) + \left(19451\ \frac{lb}{hr}\ propylene\right)\left(\frac{1\ lbmol}{42.08\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ propylene}\right)$$
$$+ \left(1901\ \frac{lb}{hr} acrylic\ acid\right)\left(\frac{1\ lbmol}{72.06\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ acrylic\ acid}\right) + \left(537\ \frac{lb}{hr}\ acetic\ acid\right)\left(\frac{1\ lbmol}{60.05\ lbmol}\right)\left(\frac{2\ lbmol\ carbon}{lbmol\ acetic\ acid}\right)$$
$$+ \left(58094\ \frac{lb}{hr} CO_2\right)\left(\frac{1\ lbmol}{44.01\ lbmol}\right)\left(\frac{1\ lbmol\ carbon}{lbmol\ CO_2}\right)$$

$$= 15065.7\ lbmol\ carbon$$

$$Carbon\ out = \left(162230\ \frac{lb}{hr}\ propane\right)\left(\frac{1\ lbmol}{44.1\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ propane}\right) + \left(20119\ \frac{lb}{hr}\ propylene\right)\left(\frac{1\ lbmol}{42.08\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ propylene}\right)$$
$$+ \left(28548\ \frac{lb}{hr} acrylic\ acid\right)\left(\frac{1\ lbmol}{72.06\ lbmol}\right)\left(\frac{3\ lbmol\ carbon}{lbmol\ acrylic\ acid}\right) + \left(1393\ \frac{lb}{hr}\ acetic\ acid\right)\left(\frac{1\ lbmol}{60.05\ lbmol}\right)\left(\frac{2\ lbmol\ carbon}{lbmol\ acetic\ acid}\right)$$
$$+ \left(59894\ \frac{lb}{hr} CO_2\right)\left(\frac{1\ lbmol}{44.01\ lbmol}\right)\left(\frac{1\ lbmol\ carbon}{lbmol\ CO_2}\right)$$

$$= 15066.2\ lbmol\ carbon$$

$$\%Error = \frac{15066.2 - 15065.7}{15066.2} \times 100\% = .\mathbf{0034}\%$$

Reactor Sizing Calculations

$$\left(200{,}000{,}000\ \frac{lb\ acrylic\ acid}{year}\right)\left(\frac{1\ year}{7980\ hours}\right) = 25252.5\ \frac{lb}{hr}\ acrylic\ acid$$

Assume the propane to propylene conversion is *0.1*, and the propylene to acrylic acid selectivity is *0.8*

$$Propane\ required = \left(25252.5\ \frac{lb}{hr}\ acrylic\ acid\right)\left(\frac{1\ lbmol}{72.06\ \ lbmol}\right)\left(\frac{1\ lbmol\ propylene}{0.8\ lbmol\ acrylic\ acid}\right)\left(\frac{1\ lbmol\ propane}{0.1\ lbmol\ propylene}\right)\left(\frac{44.1\ lb\ propane}{lbmol\ propane}\right)$$

$$= \mathbf{193176.2\ lb\ propane}$$

$$Oxygen\ required\ (stoich) = \left(25252.5\ \frac{lb}{hr}\ acrylic\ acid\right)\left(\frac{1\ lbmol}{72.06\ lbmol}\right)\left(\frac{2\ lbmol\ O_2}{lbmol\ propane}\right)\left(\frac{32.0\ lb\ O_2}{lbmol\ O_2}\right)$$

$$= \mathbf{22428\ lb\ O_2}$$

Due to acrylic acid, nitrogen, and other components flowing through the recycle, actual propane flow rate is *180250 lb/hr*, and total flow is *620230 lb/hr* or *1,160,000* ft^3/hr.

Target space velocity τ= *1700* hr^{-1}

$$Reactor\ volume = \frac{Q}{\tau} = \frac{1160000\ \frac{ft^3}{hr}}{1700\ hr^{-1}} = \mathbf{682.3\ ft^3}\ (minimum)$$

Choose 4000 tubes, pipe diameter of 2 in, length of 8 ft.

$$Actual\ Reactor\ Volume = (\#\ tubes)(\pi r^2 L) = \mathbf{698.1\ ft^3}$$

$$Cross\ Sect.Area\ (A_c) = (\#\ tubes)(\pi r^2) = \ 87.3\ \text{ft}^2$$

$$Surface\ Area\ (A_s) = (\#\ tubes)(\pi dL) = \ 16755.2\ \text{ft}^2$$

$$Superficial\ velocity\ (u_0) = \frac{Q}{A_c} = 13{,}287\ \frac{ft}{hr} = \mathbf{3.69}\ \boldsymbol{\frac{ft}{s}}$$

Using estimated catalyst properties such as space velocity from US Patent #8,193,387, the mass of the catalyst required was calculated to be 72,705 grams.

$$\left(\text{Propane to Reactor in } \frac{\text{lbmol}}{\text{hr}}\right)\left(\frac{\text{Molecular weight of Propane}}{\left(\frac{\text{mass propane}}{\text{mass catalyst}}\right)}\right) = \text{mass of catalyst required}$$

$$\left(4093\ \frac{\text{lbmol}}{\text{hr}}\right)\left(\frac{44.1\frac{\text{grams propane}}{\text{lbmol}}}{2.48\ \frac{\text{grams propane}}{\text{grams catalyst}}}\right) \cong 72{,}705 \text{ grams of catalyst}$$

Density of catalyst estimated to be that of bismuth molybdate.

$$V_{cat} = \frac{M_{cat}}{\rho_{cat}} = \frac{72705\ g}{5.95\ \frac{g}{cm^3}} = 12219\ cm^3 = \mathbf{0.432}\ \boldsymbol{ft^3}$$

Reactor Pressure Drop

Tube side pressure drop calculated using Ergun Equation, assuming a bed voidage of 0.4. Dynamic viscosity (μ) assumed $5x10^{-5}\ Pa^{-1}$. Particle diameter assumed *0.025 ft* Calculations conducted in metric units.

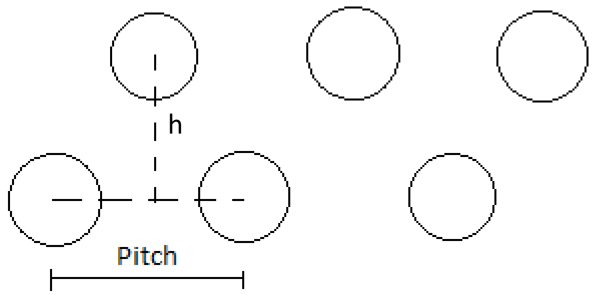
$$-\Delta P = \frac{150 u_0 \mu L(1-\varepsilon)^2}{{D_p}^2\varepsilon^3} + 1.75\frac{{u_0}^2 L(1-\varepsilon)\rho}{D_p\varepsilon^3}$$

$$= \frac{150\left(1.12\frac{m}{s}\right)(5\times10^{-5}Pa^{-1})(2.44\ m)\left(1-(0.4)\right)^2}{(0.00762\ m)^2(0.4)^3} + 1.75\frac{\left(1.12\frac{m}{s}\right)^2(2.44\ m)\left(1-(0.4)\right)\left(5.91\frac{kg}{m^3}\right)}{(0.00762\ ft)(0.4)^3}$$

$$= \mathbf{41303.1}\ \boldsymbol{Pa} = \mathbf{5.99}\ \boldsymbol{psi}$$

Shell Sizing Calculation

Assume triangular pitch tube arrangement, with 3 tubes comprising an equilateral triangle and each pitch equal to 1.25 times the outer diameter. Also assume area between equilateral triangles is equivalent to 2 equilateral triangles, so that the total tube spacing area is 3 times this value.



$$Pitch = (1.25) \times (O.D.) = (1.25)(2.37\ in) = 2.96\ in$$
$$h = \sqrt{Pitch^2 - \left(\frac{Pitch}{2}\right)^2} = 2.56\ in$$
$$Area = \frac{(Pitch)(h)}{2} = 3.79\ in^2$$
$$Spacing\ area = 3 \times Area = 11.38\ in^2$$

We would need 4000 tubes / 3 or 1334 equilateral triangles

$$Shell\ area = (1334\ tubes) \times (11.38\ in^2) = 15181\ in^2$$

If overall shell surface area is circular in shape, to meet this cross sectional area,

$$Shell\ diameter = 2\sqrt{\frac{15181\ in^2}{\pi}} = \mathbf{139.0\ in}$$

Due to the large diameter, it may be advisable to separate the tubes into multiple smaller shells.

Heat Transfer Surface Area

Required heat removal from reactor is *Q = 118,000,000 Btu/hr* (to maintain a no more than 40 °F temperature increase across the reactor) and assuming *100°F*.

$$A_s = \frac{Q}{\Delta T_{lm} U} = \frac{1.18 \times 10^8 \frac{Btu}{hr}}{(100°F)\left(100\ \frac{Btu}{hr \cdot ft^2}\right)} = \mathbf{11{,}800\ ft^2\ minimum}$$
$$Actual\ surface\ area = 16{,}755.2\ ft^2 > 11{,}800\ ft^2$$

Reactor Costing

The bare module cost is the product of the base cost (C_B) and the pressure (F_P), material (F_M), length (F_L) and bare module (F_B) factors.

$$C_P = (F_P F_M F_L + F_B) C_B$$
$$F_P = 1\ (for\ shell\ pressure < 100\ psig)$$
$$F_M = a + \left(\frac{A}{100}\right)^b = 1.75 + \left(\frac{16755.2\ ft^2}{100}\right)^{0.13} = 3.70\ (for\ stainless\ steel)$$
$$F_L = 1.25\ (for\ tube\ length\ of\ 8\ ft)$$

$$C_B = \exp\{11.2927 - 0.9228[ln(A)] + 0.09861[\ln(A)]^2\} = \$114{,}236$$

$$C_P = [(1.00)(3.70)(1.25) + (3.21))](\$114{,}236) = \$\mathbf{895,040}$$

Sample Catalyst Price Calculation

Since the mixed metal oxide catalyst is not commercial available, the price of bismuth molybdate per gram ($3.76) times a factor of 3 was used to estimate the cost. Thus, the fixed bed reactor will be using $820,109 worth of catalyst every two years. It is estimated that 15% of the catalyst can be sold back as raw materials. Thus, if the lifetime of the plant is estimated to be 16 years, the catalyst will be needed to be purchased 8 times resulting in the total cost of the catalyst to be $5,576,741.

$$(\text{g of catalyst}) * \left(\frac{\$}{\text{g ofcatalyst per 2 years}}\right) * \text{ factor} * \text{ years of operation} * (1 - \text{fraction recovered}) \cong \text{total cost of catalyst}$$

$$(72{,}705\ grams\ of\ catalyst) * \left(\frac{\$3.76}{gram\ of catalyst\ per\ 2\ years}\right) * 3 * 16\ years * (1 - .15) \cong \$5{,}576{,}741$$

Dowtherm A Mass and Price Calculation

Mass

Required heat removal from reactor (R-101) = Q = 118,000,000 Btu/hr

Specific Heat Capacity of Dowtherm A = C_P = 2.25 Btu/kg-K

Temperature increase of Dowtherm A (assumed/allowed) = ΔT = 300 K

Q = $mC_P\Delta T$ → m = Q/($C_P\Delta T$) = 175,000 kg/hr = **385,000 lb/hr**

Price

Unit Cost of DowthermA = $4,000 per metric ton

Mass of Dowtherm A required = 175,000 kg = 175 metric tons

Cost of Dowtherm A = ($4,000)*(175) = **$700,000**

Sample Cooling Water Requirement Calculation (for HX-104)

Required heat removal = Q = 63,053,511 Btu/hr

$T_{C\text{-}IN}$ = 75°F

$T_{C\text{-}OUT}$ = 95°F

Specific Heat Capacity of Water (avg over temperature range) = C_P = 0.99825 Btu/lb-°F

Q = $mC_P\Delta T$ → m = Q/($C_P\Delta T$) = **3,150,000 lb/hr**

Sample Reaction Vessel Price Calculation

A sample calculation to determine the size and price of distillation column D-101 was performed. All referenced equations come from Chapters 19 to 22 of *Seider, Seader, Lewin, Widagdo.*

Properties from Aspen for D-101

Tray Temperature	318^{o}F
Vapor Density	2.18x10^{-3} lbmol/ft^3
Vapor Flow	1071 lbmol/hr = 23.5 lb/s
Liquid Flow	1169 lbmol/hr
Liquid Density	.45 lbmol/ft^3
Liquid Surface Tension	2.01 dyne/cm
Reflux Ratio:	3.5

Flooding Velocity:

$$F_{ST} = (\frac{\sigma}{20})^{.2} = (\frac{2.01}{20})^{.2} = 0.63\ \frac{dyne}{cm}$$

$$F_{LG} = \frac{L}{G}(\frac{\rho_v}{\rho_l})^{.5} = \frac{1169\frac{lbmol}{hr}}{1071\frac{lbmol}{hr}}(\frac{2.18x10^{-3}\ lbmol/ft^3}{.45\ lbmol/ft^3})^{\frac{1}{2}} = 0.084$$

$$C_{SB} = 0.21\ \frac{ft}{s}$$

$$F_f = 1.0$$

$$F_{HA} = 1.0$$

$$U_f = C_{SB}F_{ST}F_F F_{HA}(\frac{\rho_L - \rho_v}{\rho_v})^{\frac{1}{2}}$$

$$U_f = (0.24) * (0.8) * (1) * (1) * (\frac{0.45\frac{lbmol}{ft^3} - 2.18x10^{-3}\ lbmol/ft^3}{2.18x10^{-3}\ lbmol/ft^3})^{\frac{1}{2}}$$

$$U_f = 1.9\ ft/s$$

$$U = 0.85 * U_f = 1.61\ ft/s$$

Diameter of Tower:

$$D = \frac{4V}{.9\pi\rho_v U}^{\frac{1}{2}} = \left(\frac{4 * \left(0.3\frac{lbmol}{s}\right)}{.9 * \pi * 2.18x10^{-3}\frac{lbmol}{ft^3} * 1.61\frac{ft}{s}}\right)^{\frac{1}{2}} = 11.2 \approx 12\ feet$$

Height of Tower:

$$H = (HeadSpace) + \left(N_{trays} - 1\right) * (TraySpacing) + SumpSpace$$

H= 4 ft + (19-1)*(2 ft)+10 ft = 50 ft

Pricing

Using a bare-module factor of 4.16, sieve trays ($F_{TT} = 1$), stainless steel ($F_{TM} = 2.27$), the price of the distillation tower was estimated.

Wall Thickness:

$$t_p = \frac{P_d D_i}{2SE - 1.2P_d} = \frac{(10\,psig)(12\,feet)\left(12\frac{inches}{ft}\right)}{(2*13{,}750\,psig*(1) - 1.2*10psig)}$$

$$= 0.052\,inches + 0.4375\,inches\,for\,ridgidity\,and\,corrosion = 0.4895\,inches$$

$$t_s = 0.5\,inches$$

Weight:

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

$$\mathrm{W} = \pi\left(12\text{ ft} + \frac{.5}{12}\text{feet}\right)(50\text{ ft} + 0.8*12\text{ ft}) * \left(.\frac{5}{12}\text{ft}\right)\left(490\frac{\text{lb}}{\text{ft}^3}\right) = 46{,}010\text{ lb}$$

$$C_v = e^{7.2756 - .18255(lnW) + 0.02297\ln(W)^2}$$

$$C_v = \$144{,}845$$

$$C_{PL} = 300.9*(D_i)^{0.63316}(L)^{.80161}$$

$$C_{PL} = 300.9*(12)^{0.63316}(50)^{.80161} = \$33{,}391$$

$$C_{BT} = 468\exp(0.1739*D_i) = \$3{,}772 * 19\text{ trays} = \$71{,}661$$

$$C_T = \mathrm{C_{bt}} * \frac{I}{Ib}(F_{BM} + (F_d F_b F_m - 1)$$

$$C_{BT,T} = 71{,}661 * \frac{575}{500}(4.16 + (1*1*2.27\ - 1) = \$447{,}487$$

$$C_T = C_{BT,T} + C_v * F_{BM} * \left(\frac{I}{Ib}\right)$$

$$C_{TOTAL} = \$447{,}487 + 144{,}945 * 4.16 * \left(\frac{575}{500}\right) = \mathbf{\$1{,}140{,}904}$$

Tray Efficiency Calculation

The tray efficiency for each tower was estimated to 70% from *Seider, Seader, Lewin, Widagdo*. In order to determine the accuracy of this assumption, the tray efficiency for D-103 was calculated using the equation below. The values for viscosity, temperature, K1 (acrylic acid), and K2 (water) were estimated using ASPEN. The overall efficiency was found to be approximately 66% which means that 70% efficiency was an acceptable estimate.

$$\text{Relative volatility }(\alpha) = \frac{K_1}{K_2}$$

$$\text{Tray Efficiency} = 0.492(\alpha * \mu)^{-0.245}$$

Theoretical Tray Number	Viscosity	Temperature (K)	K_1	K2	α	Stage Efficiency
1 (Condenser)	0.1848	154.9584	1.0025	0.8854	1.1323	**N/A**
2	0.1837	152.1996	1.0037	0.8724	1.1505	**72 %**
3	0.1840	152.9918	1.0049	0.8566	1.1731	**72 %**
4	0.1844	153.8825	1.0065	0.8395	1.1989	**71 %**
5	0.1850	154.9589	1.0084	0.8202	1.2295	**71 %**
6	0.1851	156.3800	1.0109	0.7974	1.2677	**71 %**
7	0.1852	158.4391	1.0144	0.7691	1.3189	**69 %**
8	0.1857	161.6806	1.0200	0.7319	1.3937	**69 %**
9	0.1864	167.1130	1.0312	0.6798	1.5169	**67 %**
10	0.1885	176.4972	1.0574	0.6002	1.7617	**64 %**
11	0.1921	186.9260	1.1172	0.5033	2.2194	**61 %**
12	0.2037	205.0980	1.4353	0.3927	3.6554	**53 %**
13	0.2091	218.8893	2.4751	0.5276	4.6912	**49 %**
14 (Reboiler)	0.2017	224.1441	3.8129	0.8037	4.7439	**N/A**
Overall Efficiency:						**66%**

Sample Heat Exchanger Size Calculation (for HX-104)

Required heat transfer = Q = 63,053,511 Btu/hr

$T_{H\text{-}IN}$ = 280°F, $T_{H\text{-}OUT}$ = 85°F

$T_{C\text{-}IN}$ = 75°F, $T_{C\text{-}OUT}$ = 95°F

$\Delta T_{LM} = [(T_{H\text{-}IN} - T_{C\text{-}OUT}) – (T_{H\text{-}OUT} - T_{C\text{-}IN})]/\ln[(T_{H\text{-}IN} - T_{C\text{-}OUT})/(T_{H\text{-}OUT} - T_{C\text{-}IN})] = 60°F$

$R = (T_{H\text{-}IN} - T_{H\text{-}OUT})/(T_{C\text{-}OUT} - T_{C\text{-}IN}) = 9.75$

$S = (T_{C\text{-}OUT} – T_{C\text{-}IN})/(T_{H\text{-}IN} - T_{C\text{-}IN}) = 0.098$

F_T = 0.98 (from Figure 18.16 in Seider, et al.)

U = 125 Btu/hr-ft^2-°F (selected from Table 18.5 in Seider, et al., for Hydrogen containing natural-gas mixtures tube side and water shell side)

$Q = UAF_T\Delta T_{LM} \rightarrow A = Q/(UF_T\Delta T_{LM})$ = **8,600 ft^2**

Cost

$F_L = 1.25$

$F_P = 1$

$F_M = 1.75 + (A/100)^{0.13} = 3.53$

$C_B = \exp[11.2927 – 0.9228*\ln(A) + .09861*\ln(A)^2]$ = \$61,500

$C_P = F_PF_MF_LC_B$ = **\$272,000**

Complete Heat Exchanger Size Calculation for HX-107

A heat exchanger is sized using a number of equations. First, a heat-transfer coefficient is estimated. Assuming a countercurrent heat exchanger, $F_T\{R,S\}=1$. The area of heat transfer is estimated using the equation:

$$A_D = \frac{Q}{U_D \Delta T_{LM} \mathrm{FT}\{\mathrm{R,S}\}}$$

Where Q is the calculated heat transfer throughout the system, U is the heat-transfer coefficient, and T_{LM} is the log mean temperature difference.

The cross-sectional area of the system then determined, in order to calculate the number of tubes/pass:

$$A_{ci} = \frac{m_i}{\rho_i u_i}$$

$$N_t = \frac{4A_{ci}}{\pi D_i^2}$$

Where m is the mass flowrate, ρ is the density, and u is the velocity. D_i is the inner diameter of the tube.

After a tube length is selected, the area of one tube and the number of tube passes is determined:

$$A_t = \pi D_0 L$$

$$N_p = \frac{A_D}{A_t N_t}$$

Where D_0 is the external diameter of the tube. The length of the tubes are adjusted until N_p is an integer.

Once a friction modifier is selected, h_i, h_o, and U are calculated:

$$h_o = N_{Re} \frac{k_o}{D_e}$$

Where N_{Re} is the Reynold's number, k_o is the thermoconductivity constant, and D_e is the effective diameter.

$$h_i = \frac{k_i}{D_i} N_{Nu}$$

Where k is the thermoconductivity constant, D is the inner diameter, and N_{Nu} is the Nusselt number.

$$\frac{1}{U} = (\frac{1}{h_i} + \frac{1}{h_o})$$

Once the calculated heat-transfer coefficient is found, it is used in place of the estimate from the beginning of the calculations, and the loop begins again.

Using this method, it was found that HX-107 has a heat transfer coefficient of 78.2 BTU/°F·ft^2·hr, 1 tube/pass, about 8 passes/tube (with an assumed tube length of 16 ft). Calculations can be seen below:

Mass Flow Rate outer	123733.8	lb/hr
Mass Flow Rate outer	34.4	lb/s
Tc, in	75	degrees F
Tc, out	95	degrees F
Th, in	415	degrees F
Th, out	100	degrees F
Di	4	in
Di	0.333333333	ft
Do	4.5	in
Do	0.375	ft
Cp (avg) hot stream	0.46	Btu/lb.F
Cp (avg) cold stream	0.5	Btu/lb.F
Density (avg) cold stream	62.4	lb/ft^3
Density (avg) hot stream	50	lb/ft^3
mu (avg) hot stream	0.000268788	lb/ft.s
mu (avg) cold stream	0.00001791	lb/ft.s
k (avg) hot stream	0.28305	Btu/(hr.ft.F)
k (avg) hot stream	0.000078625	Btu/(s.ft.F)
k (avg) cold stream	0.3566	Btu/(hr.ft.F)
k (avg) cold stream	9.90556E-05	Btu/(s.ft.F)
Fouling Factor	0.004	hr. ft^3.F/Btu
Q	343.705	Btu/s
U (guess 1)	78	Btu/(F. ft^2.hr)
U (guess 1)	0.021666667	Btu/(F. ft^2.s)
Ft(R,S)	1	
dT (LM)	115.7	
Ao	137.09	ft^2
u (known)	1.607	ft/s
volumetric flow	505.1	ft^3/hr
Mass Flow Rate inner	7.024	lb/s
Aci	0.09	ft^2
Nt	1.00	tubes/pass
L (guess 1)	16	ft

At	16.76	ft^2
Np	8.17	passes
R	0.06	
S	0.93	
Ft(R,S)	0.88	
Ao	156.5	ft^2
Np	9.3	passes
b_max	2.58	ft
b_min	0.52	ft
b (guess)	1.666666667	ft
G_inner	80.35	lb/s. ft^2
Nu_inner	93.03	
h_inner	78.99	Btu/(hr. ft^2.F)
Pitch	0.47	ft
C	0.09	ft
Acf	0.19	ft^2
G_outer	646608.89	lb/hr.ft^2
De	0.37	ft
Nu_outer	3721027.73	
Np_outer	325.45	
N_Nu	10178.03	
h_outer	7764.39	Btu/(hr. ft^2.F)
U_1	78.20	Btu/(F. ft^2/hr)
U_guess	78	Btu/(F. ft^2.hr)

Sample Condenser Calculation

Condensers were sized the same as heat exchangers with:

$$A_c = \frac{Q_C}{U\Delta T_{LM}}$$

The purchase cost for each condenser was determined from:

$$C_p = F_P F_M F_L C_B$$

with

$$F_P = 0.9803 + 0.018\left(\frac{P}{100}\right) + 0.0017 * \left(\frac{P}{100}\right)^{\frac{1}{2}}$$

$$F_M = a + (\frac{SA}{100})^b$$

where a and b are material factors. F_L is a tube length correction factor. C_b for a fixed-head is

$$C_b = \exp\{11.2927 - 0.9228[lnA] + 0.9861[lnA]^2$$

Sample Reboilers Calculation

The reboilers were sized by the equation:

$$A_R = \frac{Q_R}{Flux}$$

The purchase cost for each reboiler was determined using the following equation for a kettle vaporizer:

$$C_b = \exp\{12.202 - 0.8709[lnA] + 0.09005[lnA]^2$$

Sample Reflux Accumulator Calculation

In order to size the reflux accumulators, the following equations were used. This is an example calculation for the reflux accumulator in distillation tower D-101.

$$v_{drum,in} = (1+R)(D_{volumeric}) = (1+3.5)\left(286.3\frac{ft^3}{hr}\right) = 1{,}288.5\ \frac{ft^3}{hr}$$

For a residence time = 5 minutes at half full:

$$Volume = v_{drum,in} * (\,residence\ time) = 1{,}288.5\ \frac{ft^3}{hr} * \left(\frac{5\ min}{\frac{60min}{hr}}\right) * 2 = 214.7\ ft^3$$

For L/D = 3

$$V = \pi(\frac{D}{2})^2 L$$

$$D = (\frac{\frac{4}{3}V}{\pi})^{\frac{1}{3}} = (\frac{\frac{4}{3}V}{\pi})^{\frac{1}{3}} = 4.5\ ft$$

$$L = 13.5\ ft$$

The reflux accumulator is costed as a horizontal pressure vessel of carbon steel with a design pressure of 10 psig.

Wall Thickness:

$$t_p = \frac{P_d D_i}{2SE - 1.2P_d} = \frac{(10\ psig)(12\ feet)\left(12\frac{inches}{ft}\right)}{(2 * 13{,}750\ psig * (1) - 1.2 * 10 psig)}$$

$$= 0.052\ inches + 0.4375\ inches\ for\ ridgidity\ and\ corrosion = 0.4895\ inches$$

$$t_s = 0.5\ inches$$

Weight:

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

$$\mathrm{W} = \pi\left(4.5\ \mathrm{ft} + \frac{.5}{12}\mathrm{feet}\right)(13.5\ \mathrm{ft} + 0.8 * 4.5\ \mathrm{ft}) * \left(.\frac{5}{12}\mathrm{ft}\right)\left(490\frac{\mathrm{lb}}{\mathrm{ft}^3}\right) = 4{,}981\ \mathrm{lb}$$

$$C_v = e^{8.9552 - .2330(lnW) + 0.04333\ \ln(W)^2}$$

$$C_v = \$24{,}507$$

$$C_{PL} = 2005 * (D_i)^{0.20294}$$

$$C_{PL} = \$2{,}721$$

$$C_P = (\mathrm{C_{pl}} + \mathrm{F_M} * \mathrm{C_v}) * \frac{I}{Ib}$$

$$C_P = (\$2{,}721 + (1) * 24{,}507) * \left(\frac{575}{500}\right) = \$31{,}312$$

$$C_{TOTAL} = (3.05) * \$31{,}312 = \$95{,}502$$

Sample Compressor/Turbine Calculation for C-101

The price of the compressor is determined by the equation:

$$C_P = F_D F_M C_B$$

Where F_D is the drive factor, F_M is the material factor, and C_B is the base purchase cost.
F_D=1.25
F_M=1
C_B=exp(7.58 + 0.8*ln(power))
Power=9,293 hp
C_B=$2,927,365
C_P=$3,871,440 (in 2006 currency), $3,659,206 (in 2012 currency)

Sample Pump Calculation for P-101

The amount of work required to power the pump is calculated using:

$$\dot{W} = Fv(\Delta P)\frac{1}{efficiency}$$

Where F is the molar flowrate, v is the molar volume, and ΔP is the pressure change.

$$\dot{W} = \frac{1402.2\ \frac{lbmol}{hr} * 0.58108\ \frac{ft^3}{hr} * 18{,}000\ psfa}{3600\frac{sec}{hr}} * 1\frac{hp}{550\frac{ft\cdot lb_f}{sec}} * \frac{1}{.5375} = 13.78\ hp$$

$$= 10.276\ kW$$

The pump head is calculated using:

$$H = \left(\frac{V_d^2}{2g} + z_d + \frac{P_d}{\rho_d g}\right) - \left(\frac{V_s^2}{2g} + z_s + \frac{P_s}{\rho_s g}\right)$$

Where V is the velocity, g is the gravitational constant, z is the elevation, P is the pressure, ρ is the density, subscript 'd' is the discharge stream and subscript 's' is the suction stream. The velocity, height, and density are assumed to be constant, so the pump head is determined by:

$$H = \frac{1}{\rho g}(P_d - P_s)$$

$$H = \frac{1}{59.6\ \frac{lb}{ft^3} * 32.2\ \frac{ft}{sec^2}}(21{,}600\ psfa - 3600\ psfa) = 9.37\ ft$$

Aspen also reports pump head in units of $ft\text{-}lb_f/lb_m$, in which case pump head does not have the gravitational term:

$$H = \frac{1}{\rho}(P_d - P_s) = \frac{18{,}000\ psfa}{59.6\ \frac{lb}{ft^3}} = 301.8\ ft\frac{lb_f}{lb_m}$$

Cost

The price of the pump is determined by:

$$C_p = F_T F_M C_B$$

Where F_T is the type factor, F_M is the material factor, and C_B is the base cost.

F_T=1

F_M=2

C_B=exp(9.7171-0.6019*ln(s)+0.0519*ln(S)^2)

S=Q*(H)$^{0.5}$

S=1762

C_B=$3353

C_P=$6,706 (in 2006 currency), $7,712 (in 2012 currency)

Sample Storage Tank Costing Calculation

For the product in a cone roof storage tank, it is assumed 1 week's worth of propane will be stored onsite to mitigate uncertainties in shipment.

$$V_{stor} = (12\ hours)$$
$$= \left(393.5\ \frac{ft^3}{hr}\right)\left(\frac{24\ hours}{1\ day}\right)\left(\frac{7\ days}{1\ week}\right)\left(\frac{7.48\ gal}{1\ ft^3}\right) = 493860\ gallons\ minimum$$
$$Actual\ volume = 700000 gal$$
$$C_P = 265 V^{0.51} = (265)(700000\ gal)^{0.51} = \$\mathbf{253,656}$$

Appendix D: Economic Analysis Results

Seider et al. Spreadsheets

General Information

Process Title:	**Propane to Acrylic Acid**
Product:	**Acrylic Acid**
Plant Site Location:	**U.S. Gulf Coast**
Site Factor:	**1.00**
Operating Hours per Year:	**7920**
Operating Days Per Year:	**330**
Operating Factor:	**0.9041**

Product Information

This Process will Yield

	25,253	lb of Acrylic Acid per hour
	606,061	lb of Acrylic Acid per day
	200,000,000	lb of Acrylic Acid per year
Price	**$1.75**	**/lb**

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 5 year MACRS	Product Price
2013	Design		0.0%		
2014	Construction	100%	0.0%		
2015	Production	0%	45.0%	20.00%	$1.75
2016	Production	0%	67.5%	32.00%	$1.75
2017	Production	0%	90.0%	19.20%	$1.75
2018	Production		90.0%	11.52%	$1.75
2019	Production		90.0%	11.52%	$1.75
2020	Production		90.0%	5.76%	$1.75
2021	Production		90.0%		$1.75
2022	Production		90.0%		$1.75
2023	Production		90.0%		$1.75
2024	Production		90.0%		$1.75
2025	Production		90.0%		$1.75
2026	Production		90.0%		$1.75
2027	Production		90.0%		$1.75
2028	Production		90.0%		$1.75
2029	Production		90.0%		$1.75

Raw Materials

	Raw Material:	Unit:	Required Ratio:		Cost of Raw Material:	
1	Propane	lb	0.9574902	lb per lb of Acrylic Acid	$0.213	per lb
2	Compressed Oxygen	lb	0.964921	lb per lb of Acrylic Acid	$0.03	per lb
	Total Weighted Average:				$0.233	per lb of Acrylic Acid

Byproducts

	Byproduct:	Unit:	Ratio to Product		Byproduct Selling Price	
1	Wastewater	lb	0.7409505	lb per lb of Acrylic Acid	-$5.105E-02	per lb
	Total Weighted Average:				-$3.782E-02	per lb of Acrylic Acid

Utilities

	Utility:	Unit:	Required Ratio		Utility Cost	
1	High Pressure Steam	lb	0.6337	lb per lb of Acrylic Acid	$0.012	per lb
2	Low Pressure Steam	lb	2.6066	lb per lb of Acrylic Acid	$8.295E-03	per lb
3	Process Water	gal	0	gal per lb of Acrylic Acid	$0.000E+00	per gal
4	Cooling Water	gal	47.550623	gal per lb of Acrylic Acid	$1.250E-04	per gal
5	Electricity	kWh	0.7302603	kWh per lb of Acrylic Acid	$0.069	per kWh
	Total Weighted Average:				$0.086	per lb of Acrylic Acid

Variable Costs

General Expenses:

Selling / Transfer Expenses:	**3.00%**	**Of Sales**
Direct Research:	**4.80%**	**of Sales**
Allocated Research:	**0.50%**	**of Sales**
Administrative Expense:	**2.00%**	**of Sales**
Management Incentive Compensation:	**1.25%**	**of Sales**

Working Capital

Accounts Receivable	**30**	**Days**
Cash Reserves (excluding Raw Materials)	**30**	**Days**
Accounts Payable	**30**	**Days**
Acrylic Acid Inventory	**7**	**Days**
Raw Materials	**2**	**Days**

Total Permanent Investment

Cost of Site Preparations:	**5.00%**	**of Total Bare Module Costs**
Cost of Service Facilities:	**5.00%**	**of Total Bare Module Costs**
Allocated Costs for utility plants and related facilities:	**$0**	
Cost of Contingencies and Contractor Fees:	**18.00%**	**of Direct Permanent Investment**
Cost of Land:	**2.00%**	**of Total Depreciable Capital**
Cost of Royalties:	**$0**	
Cost of Plant Start-Up:	**10.00%**	**of Total Depreciable Capital**

Fixed Costs

Operations

Operators per Shift:	**6**	**(assuming 5 shifts)**
Direct Wages and Benefits:	**$40**	**/operator hour**
Direct Salaries and Benefits:	**30%**	**of Direct Wages and Benefits**
Operating Supplies and Services:	**6%**	**of Direct Wages and Benefits**
Technical Assistance to Manufacturing:	**$150,000.00**	**per year, for each Operator per Shift**
Control Laboratory:	**$150,000.00**	**per year, for each Operator per Shift**

Maintenance

Wages and Benefits:	**4.50%**	**of Total Depreciable Capital**
Salaries and Benefits:	**25%**	**of Maintenance Wages and Benefits**
Materials and Services:	**100%**	**of Maintenance Wages and Benefits**
Maintenance Overhead:	**5%**	**of Maintenance Wages and Benefits**

Operating Overhead

General Plant Overhead:	**7.50%**	**of Maintenance and Operations Wages and Benefits**
Mechanical Department Services:	**3.00%**	**of Maintenance and Operations Wages and Benefits**
Employee Relations Department:	**6.00%**	**of Maintenance and Operations Wages and Benefits**
Business Services:	**7.40%**	**of Maintenance and Operations Wages and Benefits**

Property Taxes and Insurance

Property Taxes and Insurance:	**3%**	**of Total Depreciable Capital**

Straight Line Depreciation

Direct Plant:	8.00%	**of Total Depreciable Capital, less 1.18 times the Allocated Costs for Utility Plants and Related Facilities**
Allocated Plant:	6.00%	**of 1.18 times the Allocated Costs for Utility Plants and Related Facilities**

Other Annual Expenses

Rental Fees (Office and Laboratory Space):	**$0**
Licensing Fees:	**$0**
Miscellaneous:	**$0**

Depletion Allowance

Annual Depletion Allowance:	**$0**

Variable Cost Summary

Variable Costs at 100% Capacity:

General Expenses

	Selling / Transfer Expenses:		$ 10,500,000
	Direct Research:		$ 16,800,000
	Allocated Research:		$ 1,750,000
	Administrative Expense:		$ 7,000,000
	Management Incentive Compensation:		$ 4,375,000
Total General Expenses			$ 40,425,000
Raw Materials	$0.232893	per lb of Acrylic Acid	$46,578,610
Byproducts	-$0.037823	per lb of Acrylic Acid	$7,564,660
Utilities	$0.085684	per lb of Acrylic Acid	$17,136,845
Total Variable Costs			**$ 111,705,115**

Fixed Cost Summary			
Operations			
	Direct Wages and Benefits	$	2,496,000
	Direct Salaries and Benefits	$	748,800
	Operating Supplies and Services	$	149,760
	Technical Assistance to Manufacturing	$	4,500,000
	Control Laboratory	$	4,500,000
	Total Operations	**$**	**12,394,560**
Maintenance			
	Wages and Benefits	$	3,048,511
	Salaries and Benefits	$	762,128
	Materials and Services	$	3,048,511
	Maintenance Overhead	$	152,426
	Total Maintenance	**$**	**7,011,574**
Operating Overhead			
	General Plant Overhead:	$	529,158
	Mechanical Department Services:	$	211,663
	Employee Relations Department:	$	423,326
	Business Services:	$	522,102
	Total Operating Overhead	**$**	**1,686,250**
Property Taxes and Insurance			
	Property Taxes and Insurance:	$	2,032,340
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	$	-
	Licensing Fees:	$	-
	Miscellaneous:	$	-
	Total Other Annual Expenses	**$**	**-**
Total Fixed Costs		**$**	**23,124,724**

Investment Summary

Bare Module Costs		
Fabricated Equipment	$ -	
Process Machinery	$ 41,454,717	
Spares	$ 3,629,192	
Storage	$ 831,406	
Other Equipment	$ 699,530	
Catalysts	$ 5,576,741	
Computers, Software, Etc.	$ -	
Total Bare Module Costs:		**$ 52,191,586**
Direct Permanent Investment		
Cost of Site Preparations:	$ 2,609,579	
Cost of Service Facilities:	$ 2,609,579	
Allocated Costs for utility plants and related facilities:	$ -	
Direct Permanent Investment		**$ 57,410,744**
Total Depreciable Capital		
Cost of Contingencies & Contractor Fees	$ 10,333,934	
Total Depreciable Capital		**$ 67,744,678**
Total Permanent Investment		
Cost of Land:	$ 1,354,894	
Cost of Royalties:	$ -	
Cost of Plant Start-Up:	$ 6,774,468	
Total Permanent Investment - Unadjusted		$ 75,874,040
Site Factor		1.00
Total Permanent Investment		**$ 75,874,040**

Working Capital

	2014	2015	2016
Accounts Receivable	$ 12,945,205	$ 6,472,603	$ 6,472,603
Cash Reserves	$ 1,489,127	$ 744,563	$ 744,563
Accounts Payable	$ (2,356,599)	$ (1,178,300)	$ (1,178,300)
Acrylic Acid Inventory	$ 3,020,548	$ 1,510,274	$ 1,510,274
Raw Materials	$ 114,851	$ 57,426	$ 57,426
Total	**$ 15,213,132**	**$ 7,606,566**	**$ 7,606,566**
Present Value at 15%	*$ 13,228,811*	*$ 5,751,657*	*$ 5,001,441*

Total Capital Investment **$ 99,855,948**

Profitability Measures

The Internal Rate of Return (IRR) for this project is 84.92%

The Net Present Value (NPV) of this project in 2013 is $ 384,963,400

ROI Analysis (Third Production Year)

Annual Sales	**315,000,000**	
Annual Costs	**(133,749,929)**	
Depreciation	**(6,069,923)**	
Income Tax	**(64,816,655)**	
Net Earnings	**110,363,493**	
Total Capital Investment		**106,300,304**
ROI	**103.82%**	

Appendix E: Material Safety Data Sheets (MSDS)

Material Safety Data Sheet

Propane

~~Section 1. Chemical product and company identification~~

Product name : Propane

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

Product use : Synthetic/Analytical chemistry.

Synonym : n-Propane; Dimethylmethane; Freon 290; Liquefied petroleum gas; Lpg; Propyl hydride; R 290; C3H8; UN 1075; UN 1978; A-108; Hydrocarbon propellant.

MSDS # : 001045

Date of Preparation/Revision : **4/26/2011.**

Incaseofemergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS LIQUEFIED COMPRESSED GAS; ODORLESS BUT MAY HAVE SKUNK ODOR ADDED.]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Target organs : May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).

Routes of entry : Inhalation

Potentialacutehealtheffects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Acts as a simple asphyxiant.

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

Potentialchronichealtheffects

Chronic effects : May cause target organ damage, based on animal data.

Target organs : May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).

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

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

Name	CASnumber	%Volume	Exposurelimits
Propane	74-98-6	100	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1800 mg/m³ 10 hour(s). TWA: 1000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s).

Section 4. First aid measures

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

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

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

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

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

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

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 450°C (842°F)

Flash point : Closed cup: -104°C (-155.2°F). Open cup: -104°C (-155.2°F).

Flammable limits : Lower: 2.1% Upper: 9.5%

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

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

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

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

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

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

Section 6. Accidental release measures

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

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

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

Section 7. Handling and storage

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

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

Section 8. Exposure controls/personal protection

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

Personalprotection

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

Respiratory : 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.

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

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

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

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Productname

Propane	**ACGIH TLV (United States, 2/2010).** TWA: 1000 ppm 8 hour(s). **NIOSH REL (United States, 6/2009).** TWA: 1800 mg/m³ 10 hour(s). TWA: 1000 ppm 10 hour(s). **OSHA PEL (United States, 6/2010).** TWA: 1800 mg/m³ 8 hour(s). TWA: 1000 ppm 8 hour(s). **OSHA PEL 1989 (United States, 3/1989).** TWA: 1800 mg/m³ 8 hour(s).

TWA: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight Molecular	: 44.11 g/mole
formula	: C3-H8
Boiling/condensation point	: -42°C (-43.6°F)
Melting/freezing point	: -189.7°C (-309.5°F)
Critical temperature	: 96.6°C (205.9°F)
Vapor pressure	: 109 (psig)
Vapor density	: 1.6 (Air = 1)
Specific Volume (ft^3/lb)	: 8.6206
Gas Density (lb/ft^3)	: 0.116

Section 10. Stability and reactivity

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

Section 11. Toxicological information

Toxicitydata

Product/ingredient name	Result	Species	Dose	Exposure
Propane	LC50 Inhalation Gas.	Rat	>800000 ppm	15 minutes

IDLH	: 2100 ppm
Chronic effects on humans	: May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).
Other toxic effects on humans	: No specific information is available in our database regarding the other toxic effects of this material to humans.

Specificeffects

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

Section 12. Ecological information

Aquaticecotoxicity

Not available.

Products of degradation	: Products of degradation: carbon oxides (CO, CO_2) and water.
Environmental fate	: Not available.
Environmental hazards	: This product shows a low bioaccumulation potential.
Toxicity to the environment	: Not available.

Section 13. Disposal considerations

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

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1978	PROPANE	2.1	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg **Special provisions** 19, T50
TDG Classification	UN1978	PROPANE	2.1	Not applicable (gas).		**Explosive Limitand Limited Quantity Index** 0.125 **ERAPIndex** 3000 **Passenger CarryingShip Index** 65 **Passenger Carrying RoadorRail Index** Forbidden **Special provisions** 29, 42
Mexico Classification	UN1978	PROPANE	2.1	Not applicable (gas).		-

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

Section 15. Regulatory information

UnitedStates

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

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: Propane
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Propane: Fire hazard, Sudden release of pressure

Clean Air Act (CAA) 112 accidental release prevention - Flammable Substances: Propane

Clean Air Act (CAA) 112 regulated flammable substances: Propane

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

Canada

WHMIS (Canada) : Class A: Compressed gas.
Class B-1: Flammable gas.

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

Section 16. Other information

United States

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

Canada

Label requirements : Class A: Compressed gas.
Class B-1: Flammable gas.

Propane

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

Health	*	1
Flammability		4
Physical hazards		0

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

Flammability	4
Health	1
Instability	0
Special	

Noticetoreader

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

Propylene

Section 1. Chemical product and company identification

Product name : Propylene

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

Product use : Synthetic/Analytical chemistry.

Synonym : Propene, methylethene, methylethylene, 1-propene, 1-propylene, refrigerant gas R1270

MSDS # : 001046

Date of Preparation/Revision : **5/6/2010.**

Incaseofemergency : 1-866-734-3438

Section 2. Hazards identification

Physical state : Gas. [COLORLESS LIQUEFIED COMPRESSED GAS WITH A MILD ODOR.]

Emergency overview : WARNING!

FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.

Contact with rapidly expanding gases can cause frostbite.

Routes of entry : Inhalation

Potentialacutehealtheffects

Eyes : Contact with rapidly expanding gas may cause burns or frostbite.

Skin : Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation : Acts as a simple asphyxiant.

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

Potential chronic health effects : **CARCINOGENIC EFFECTS**: A4 (Not classifiable for humans or animals.) by ACGIH, 3 (Not classifiable for humans.) by IARC.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure : Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

Name	CASnumber	%Volume	Exposurelimits
Propylene	115-07-1	100	**ACGIH TLV (United States, 1/2009).** TWA: 500 ppm 8 hour(s). **ACGIH TLV (United States, 1/2005).** TWA: 500 ppm 8 hour(s). Form: All forms

Section 4. First aid measures

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

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

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

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

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

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

Section 5. Fire-fighting measures

Flammability of the product : Flammable.

Auto-ignition temperature : 454.85 to 459.85°C (850.7 to 859.7°F)

Flash point : Closed cup: -108.15°C (-162.7°F).

Flammable limits : Lower: 2.4% Upper: 11%

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

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

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

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

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

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

Section 6. Accidental release measures

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

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

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

Section 7. Handling and storage

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

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

Section 8. Exposure controls/personal protection

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

Personalprotection

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

Respiratory : 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.

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

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

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

Personal protection in case of a large spill : Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Productname

propene	**ACGIH TLV (United States, 1/2009).** TWA: 500 ppm 8 hour(s). **ACGIH TLV (United States, 1/2005).** TWA: 500 ppm 8 hour(s). Form: All forms

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight Molecular : 42.09 g/mole

formula : C3-H6

Boiling/condensation point : -47.7°C (-53.9°F)

Melting/freezing point : -185°C (-301°F)

Critical temperature : 91.9°C (197.4°F)

Vapor pressure : 136.6 (psig)

Vapor density : 1.4 (Air = 1)

Specific Volume (ft ^{3}/lb) : 9.0909

Gas Density (lb/ft ^{3}) : 0.11

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.

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

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

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

Section 11. Toxicological information

Toxicitydata

Chronic effects on humans : **CARCINOGENIC EFFECTS**: A4 (Not classifiable for humans or animals.) by ACGIH, 3 (Not classifiable for humans.) by IARC.

Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.

Specificeffects

Carcinogenic effects : No known significant effects or critical hazards.

Mutagenic effects : No known significant effects or critical hazards.

Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquaticecotoxicity

Not available.

Products of degradation : Products of degradation: carbon oxides (CO, CO_2) and water.

Environmental fate : Not available.

Environmental hazards : No known significant effects or critical hazards.

Toxicity to the environment : Not available.

Section 13. Disposal considerations

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

Section 14. Transport information

Regulatory information	UN number	Proper shipping name	Class	Packing group	Label	Additional information
DOT Classification	UN1077	PROPYLENE SEE ALSO PETROLEUM GASES, LIQUEFIED	2.1	Not applicable (gas).		**Limited quantity** Yes. **Packaging instruction** **Passenger aircraft** Quantity limitation: Forbidden. **Cargo aircraft** Quantity limitation: 150 kg **Special provisions** 19, T50

TDG Classification	UN1077	PROPYLENE	2.1	Not applicable (gas).		**Explosive Limitand Limited Quantity Index** 0.125 **ERAPIndex** 3000 **Passenger CarryingShip Index** Forbidden **Passenger Carrying RoadorRail Index** Forbidden **Special provisions** 29
Mexico Classification	UN1077	PROPYLENE SEE ALSO PETROLEUM GASES, LIQUEFIED	2.1	Not applicable (gas).		-

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

Section 15. Regulatory information

UnitedStates

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

SARA 302/304/311/312 extremely hazardous substances: No products were found.
SARA 302/304 emergency planning and notification: No products were found.
SARA 302/304/311/312 hazardous chemicals: propene
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: propene: Fire hazard, Sudden release of pressure

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

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

Clean Air Act (CAA) 112 accidental release prevention: propene

Clean Air Act (CAA) 112 regulated flammable substances: propene

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

SARA313

	Productname	CASnumber	Concentration
Form R - Reporting requirements :	Propylene	115-07-1	100
Supplier notification :	Propylene	115-07-1	100

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

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

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

United States

Label requirements : FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
CONTENTS UNDER PRESSURE.

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.) :

Health	1
Flammability	4
Physical hazards	2

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

Flammability: 4
Health: 1
Instability: 0
Special

Noticetoreader

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

ScienceLab.com
Chemicals & Laboratory Equipment

Health	3
Fire	2
Reactivity	2
Personal Protection	

Material Safety Data Sheet
Acrylic Acid MSDS

Section 1: Chemical Product and Company Identification

Product Name: Acrylic Acid

Catalog Codes: SLA3406

CAS#: 79-10-7

RTECS: AS4375000

TSCA: TSCA 8(b) inventory: Acrylic Acid

CI#: Not available.

Synonym: Propenoic Acid Ethylenecarboxylic Acid

Chemical Name: Acrylic Acid

Chemical Formula: C3-H4-O2

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

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

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

Section 3: Hazards Identification

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

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

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

Section 4: First Aid Measures

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

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

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

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

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

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

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

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

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

Flammable Limits: Not available.

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

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

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

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

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

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

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

Section 7: Handling and Storage

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

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

Section 8: Exposure Controls/Personal Protection

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

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

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

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

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Acrid (Strong.)

Taste: Not available.

Molecular Weight: 72.06 g/mole

Color: Colorless.

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

Boiling Point: 141°C (285.8°F)

Melting Point: 14°C (57.2°F)

Critical Temperature: 342°C (647.6°F)

Specific Gravity: 1.05 (Water = 1)

Vapor Pressure: 0.5 kPa (@ 20°C)

Vapor Density: 2.5 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.092 ppm

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

Ionicity (in Water): Not available.

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

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

Section 10: Stability and Reactivity Data

Stability: The product is stable. **Instability**

Temperature: Not available. **Conditions of**

Instability: Not available. **Incompatibility**

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

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

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Yes.

Section 11: Toxicological Information

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

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

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

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

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

Section 12: Ecological Information

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

BOD5 and COD: Not available.

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

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

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 8: Corrosive material

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

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

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

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

Other Classifications:

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

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 2

Reactivity: 2

Personal Protection:

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

Health: 3

Flammability: 2

Reactivity: 2

Specific hazard:

Protective

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

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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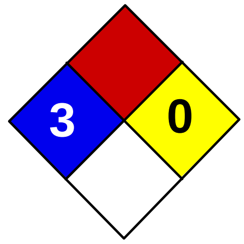

Health	3
Fire	2
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Acetic acid MSDS

Section 1: Chemical Product and Company Identification

Product Name: Acetic acid

Catalog Codes: SLA3784, SLA1438, SLA2101, SLA3604, SLA1258

CAS#: 64-19-7

RTECS: AF1225000

TSCA: TSCA 8(b) inventory: Acetic acid

CI#: Not applicable.

Synonym: Acetic acid; glacial acetic acid

Chemical Name: Acetic Acid, Glacial

Chemical Formula: C2-H4-O2

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	**CAS #**	**% by Weight**
Acetic acid	64-19-7	100

Toxicological Data on Ingredients: Acetic acid: ORAL (LD50): Acute: 3310 mg/kg [Rat]. 4960 mg/kg [Mouse]. 3530 mg/kg [Rat]. DERMAL (LD50): Acute: 1060 mg/kg [Rabbit]. VAPOR (LC50): Acute: 5620 ppm 1 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 (corrosive, permeator), of eye contact (corrosive). Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth and respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation of respiratory tract, characterized by coughing, choking, or shortness of breath. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:

Hazardous in case of skin contact (irritant), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to kidneys, mucous membranes, skin, teeth. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged contact with spray mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged exposure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection.

Section 4: First Aid Measures

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

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

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

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

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

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. 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: 463°C (865.4°F)

Flash Points: CLOSED CUP: 39°C (102.2°F). OPEN CUP: 43°C (109.4°F).

Flammable Limits: LOWER: 4% UPPER: 19.9%

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, of heat. Slightly flammable to flammable in presence of oxidizing materials, of metals.

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. Slightly explosive in presence of oxidizing materials.

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:
Reacts with metals to produces flammable hydrogen gas. It will ignite on contact with potassium-tert-butoxide. A mixture of ammonium nitrate and acetic acid ignites when warmed, especially if warmed.

Special Remarks on Explosion Hazards:

Acetic acid vapors may form explosive mixtures with air. Reactions between acetic acid and the following materials are potentially explosive: 5-azidotetrazole, bromine pentafluoride, chromium trioxide, hydrogen peroxide, potassium permanganate, sodium peroxide, and phorphorus trichloride. Dilute acetic acid and dilute hydrogen can undergo an exothermic reaction if heated, forming peracetic acid which is explosive at 110 degrees C. Reaction between chlorine trifluoride and acetic acid is very violent, sometimes explosive.

Section 6: Accidental Release Measures

Small Spill:
Dilute with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal container. If necessary: Neutralize the residue with a dilute solution of sodium carbonate.

Large Spill:
Flammable liquid. Corrosive liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. If the product is in its solid form: Use a shovel to put the material into a convenient waste disposal container. If the product is in its liquid form: Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Absorb with an inert material and put the spilled material in an appropriate waste disposal. Do not touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of sodium carbonate. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
\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, reducing agents, metals, acids, alkalis.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and

sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

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

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

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

Exposure Limits:
TWA: 10 STEL: 15 (ppm) [Australia] TWA: 25 STEL: 27 (mg/m3) [Australia] TWA: 10 STEL: 15 (ppm) from NIOSH TWA: 25 STEL: 37 (mg/m3) from NIOSH TWA: 10 STEL: 15 (ppm) [Canada] TWA: 26 STEL: 39 (mg/m3) [Canada] TWA: 25 STEL: 37 (mg/m3) TWA: 10 STEL: 15 (ppm) from ACGIH (TLV) [United States] [1999] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 25 (mg/m3) from OSHA (PEL) [United States]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Pungent, vinegar-like, sour (Strong.)

Taste: Vinegar, sour (Strong.)

Molecular Weight: 60.05 g/mole

Color: Colorless. Clear (Light.) **pH**

(1% soln/water): 2 [Acidic.] **Boiling**

Point: 118.1°C (244.6°F) **Melting**

Point: 16.6°C (61.9°F)

Critical Temperature: 321.67°C (611°F)

Specific Gravity: 1.049 (Water = 1) **Vapor**

Pressure: 1.5 kPa (@ 20°C) **Vapor**

Density: 2.07 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.48 ppm

Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -0.2

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 Glycerol, alcohol, Benzene, Carbon Tetrachloride. Practically insoluble in Carbon Disulfide.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, incompatible materials

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

Corrosivity:
Highly corrosive in presence of stainless steel(304). Slightly corrosive in presence of aluminum, of copper. Non-corrosive in presence of stainless steel(316).

Special Remarks on Reactivity:
Reacts violently with strong oxidizing agents, acetaldehyde, and acetic anhydride. Material can react with metals, strong bases, amines, carbonates, hydroxides, phosphates, many oxides,cyanides, sulfides, chromic acid, nitric acid, hydrogen peroxide, carbonates. ammonium nitrate, ammonium thiosulfate, chlorine trifluoride, chlorosulfonic acid, perchloric acid, permanganates, xylene, oleum, potassium hydroxide, sodium hydroxide, phosphorus isocyanate, ethylenediamine, ethylene imine.

Special Remarks on Corrosivity: Moderate corrosive effect on bronze. No corrosion data on brass

Polymerization: Will not occur.

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): 3310 mg/kg [Rat]. Acute dermal toxicity (LD50): 1060 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 5620 1 hours [Mouse].

Chronic Effects on Humans:
MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: kidneys, mucous membranes, skin, teeth.

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: May affect genetic material and may cause reproductive effects based on animal data. No human data found.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Extremely irritating and corrosive. Causes skin irritation (reddening and itching, inflammation). May cause blistering , tissue damage and burns. Eyes: Extremely irritating and corrosive. Causes eye irritation, lacrimation, redness, and pain. May cause burns, blurred vision, conjunctivitis, conjunctival and corneal destruction and permanent injury. Inhalation: Causes severe respiratory tract irritation. Affects the sense organs (nose, ear, eye, taste), and blood. May cause chemical pneumonitis, bronchitis, and pulmonary edema. Severe exposure may result in lung tissue damage and corrosion (ulceration) of the mucous membranes. Inhalation may also cause rhinitis, sneezing, coughing, oppressive feeling in the chest or chest pain, dyspnea, wheezing, tachypnea, cyanosis, salivation, nausea, giddiness, muscular weakness. Ingestion: Moderately toxic. Corrosive. Causes gastrointestinal tract irritation (burning and pain of the mouth, throat, and abdomen, coughing, ulceration, bleeding, nausea, abdomial spasms, vomiting, hematemesis, diarrhea. May Also affect the liver (impaired liver function), behavior (convulsions, giddines, muscular weakness), and the urinary system - kidneys (Hematuria, Albuminuria, Nephrosis, acute renal failure, acute tubular necrosis). May also cause dyspnea or asphyxia. May also lead to shock, coma and death. Chronic Potential Health Effects: Chronic exposure via ingestion may cause blackening or erosion of the teeth and jaw necrosis, pharyngitis, and gastritis. It may also behavior (similar to acute ingestion), and metabolism (weight loss). Chronic exposure via inhalation may cause asthma and/or bronchitis with cough, phlegm, and/or shortness of breath . It may also affect the blood (decreased leukocyte count), and urinary system (kidneys).

Repeated or prolonged skin contact may cause thickening, blackening, and cracking of the skin.

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 423 mg/l 24 hours [Fish (Goldfish)]. 88 ppm 96 hours [Fish (fathead minnow)]. 75 ppm 96 hours [Fish (bluegill sunfish)]. >100 ppm 96 hours [Daphnia].

BOD5 and COD: BOD-5: 0.34-0.88 g oxygen/g

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 8: Corrosive material

Identification: : Acetic Acid, Glacial UNNA: 2789 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
New York release reporting list: Acetic acid Rhode Island RTK hazardous substances: Acetic acid Pennsylvania RTK: Acetic acid Florida: Acetic acid Minnesota: Acetic acid Massachusetts RTK: Acetic acid New Jersey: Acetic acid California Director's List of Hazardous Subtances (8 CCR 339): Acetic acid TSCA 8(b) inventory: Acetic acid CERCLA: Hazardous substances.: Acetic acid: 5000 lb. (2268 kg)

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

Other Classifications:

WHMIS (Canada):
CLASS B-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):
R10- Flammable. R35- Causes severe burns. 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. S45- In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

HMIS (U.S.A.): Health

Hazard: 3

Fire Hazard: 2

Reactivity: 0

Personal Protection: H

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

Health: 3

Flammability: 2

Reactivity: 0

Specific hazard:

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

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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