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# Production of BTX from Ethane

Arthur Chen
*University of Pennsylvania*

Fiona Crowley
*University of Pennsylvania*

Jonathan Lym
*University of Pennsylvania*

Pablo Sanchez
*University of Pennsylvania*

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**Abstract**
This process will produce 0.5 MM tons of benzene, toluene, and xylene (BTX) per year from a feedstock of 0.82 MM tons of fractional-grade ethane. The conversion of ethane to BTX occurs in a steam reformer reactor operating at 1170°F, using a germanium-incorporated H-ZSM-5 zeolite catalyst. After the reaction occurs, the light components are separated from the product stream using a multistage compressor and flash followed by the PRISM separation system. The light hydrocarbons (ethylene, ethane, propylene, and propane) are recycled to the reactor and the hydrogen and methane are burned. The final BTX product is separated from the heavy stream using two distillation columns, and the remaining heavy components are sold for use in gasoline. The plant will be located on the Gulf Coast due to the abundance of fracking operations in the area, allowing for easy access to ethane feedstock and gases used in the regeneration process. The process is currently unprofitable with an IRR of 2.87% and a net present value of -$166,765,000 at a discount rate of 18%. The financials for this venture are highly sensitive to the price of catalyst components and catalyst lifetime. A few major reasons that make this venture unprofitable are the high cost of catalyst, the high equipment cost, and the short catalyst lifespan. After in depth analysis of the financials, we recommend that this project only be executed if market prices for input components significantly decrease, prices for BTX significantly increase, or catalyst lifetime significantly increases.

**Disciplines**
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

# PRODUCTION OF BTX FROM ETHANE

Design Project By:

Arthur Chen
Fiona Crowley
Jonathan Lym
Pablo Sanchez

Presented To:

Professor Leonard Fabiano
Dr. Daeyeon Lee

April 14, 2015

Department of Chemical and Biomolecular Engineering

University of Pennsylvania

School of Engineering and Applied Science

Professor Leonard Fabiano
Dr. Daeyeon Lee
University of Pennsylvania
School of Engineering and Applied Science
Department of Chemical and Biomolecular Engineering
220 S 33rd Street
Philadelphia, PA 19104

April 14, 2015

Dear Professor Fabiano and Dr. Lee,

We are pleased to present our process for the production of *BTX from Ethane* proposed by Dr. Richard Bockrath. Our plant, located along the Gulf Coast, is designed to produce 0.5 MM tons of BTX (62% Benzene, 30% Toluene, 8% Xylene) per year from 0.82 MM tons of fractional-grade ethane per year. This process utilizes the dehydroaromatization of ethane over a platinum zeolite catalyst using Group 14 elements such as germanium, tin and lead in its framework. This reaction takes place at 630$^o$C and 1 atmosphere in a furnace with packed tubes similar to the reactor used for the steam reformation of methane. The products that are leaving the reactor are separated using flash vessels, distillation units, and PRISM membrane separators. Unreacted ethane, ethylene, propane, and propylene are recycled to minimize waste and maximize conversion. Hydrogen and methane generated in this process are burned in fired furnaces to generate heat for the process. Heavier hydrocarbons that are produced are sold as a gasoline additive to maximize profits. Detailed equipment designs and a preliminary economic analysis of the plant are enclosed within.

This method of BTX production would compete with two current methods of production, namely catalytic reforming of naphtha in petroleum refineries and steam cracking of hydrocarbons. Unlike its competitors, this process uses ethane, which has become much cheaper since the shale gas boom.

We have determined that at the current prices of raw materials, products and utilities, the process would be unprofitable. Our base case currently assumes a catalyst lifespan of four weeks; however it was found that in order to have a positive Net Present Value after 15 years, the catalyst would have to be repurchased no more frequently than once every 8.5 weeks. However, provided that the market outlook is positive in the future, this plant has potential to achieve a strong hold on the emerging market.

Sincerely,

| Arthur Chen | Fiona Crowley | Jonathan Lym | Pablo Sanchez |
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# Abstract

This process will produce 0.5 MM tons of benzene, toluene, and xylene (BTX) per year from a feedstock of 0.82 MM tons of fractional-grade ethane. The conversion of ethane to BTX occurs in a steam reformer reactor operating at 1170°F, using a germanium-incorporated H-ZSM-5 zeolite catalyst. After the reaction occurs, the light components are separated from the product stream using a multistage compressor and flash followed by the PRISM separation system. The light hydrocarbons (ethylene, ethane, propylene, and propane) are recycled to the reactor and the hydrogen and methane are burned. The final BTX product is separated from the heavy stream using two distillation columns, and the remaining heavy components are sold for use in gasoline. The plant will be located on the Gulf Coast due to the abundance of fracking operations in the area, allowing for easy access to ethane feedstock and gases used in the regeneration process. The process is currently unprofitable with an IRR of 2.87% and a net present value of -$166,765,000 at a discount rate of 18%. The financials for this venture are highly sensitive to the price of catalyst components and catalyst lifetime. A few major reasons that make this venture unprofitable are the high cost of catalyst, the high equipment cost, and the short catalyst lifespan. After in depth analysis of the financials, we recommend that this project only be executed if market prices for input components significantly decrease, prices for BTX significantly increase, or catalyst lifetime significantly increases.

# Introduction and Objective-Time Chart

Due to the recent increase in fracking in the United States, there is a high availability of light paraffinic hydrocarbons to be used as feedstocks, especially ethane. While research into alkanes-to-aromatics processes was more popular in the 90s, with advances by companies such as Cyclar and Aromax, these processes fell out of favor due to the difficulty in finding a suitable catalyst. However, a recent patent by Shell showed promising conversions and selectivities to BTX for a catalyst consisting of a germanium incorporated into a zeolite.

This project is also motivated by the decrease in traditional sources of BTX, leading to a demand for new methods of production. BTX is typically made through catalytic naphtha reform or by extracting from naphtha-fed ethylene crackers, both of which require relatively expensive crude oil. As ethane is a common by-product of fracking, it is much cheaper, thus allowing for very high potential profits from this process.

Table 1. Objective Time Chart of Project Milestones

| **Completion Date** | **Milestone** |
|---|---|
| February 3 | Submit preliminary material balance and computer-drawn block flow diagram. |
| February 24 | Submit base case material balance and computer-drawn process flow diagram. |
| March 17 | Submit detailed equipment design for a key process unit. |
| March 24 | Major equipment designed. |
| March 31 | Finances completed. |
| April 7 | Written reports due. |
| April 14 | Revised written reports due. |
| April 21 | Design presentations. |

## Chemistry Background

The general reaction mechanism is shown in Figure 1. Alkanes, such as ethane and propane, undergo dehydrogenation to form alkenes. This step is the rate-limiting step for the process. The alkenes then oligomerize to form longer chain hydrocarbons. The oligomers then cyclize to form naphthenes and then are dehydrogenated to form aromatics, the final product. Hydrogen is produced throughout this process and causes the reactions to be endothermic.

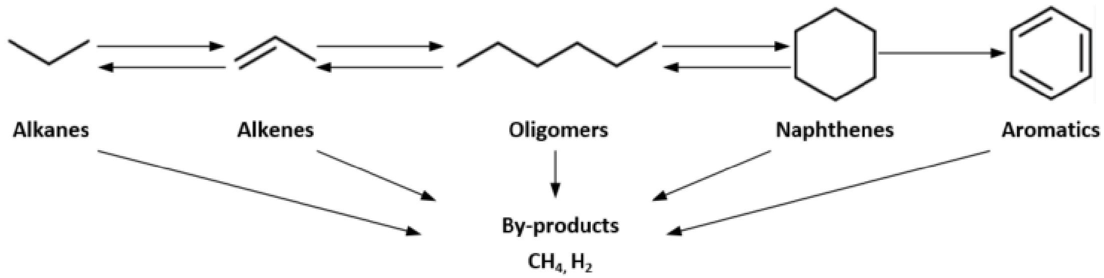


Figure 1. General mechanism for the aromatization of alkanes[1].

While the general mechanism of this process is well-known, only three stoichiometric equations of the conversion of ethane to benzene, toluene and xylene could be found[2]. Otherwise, no information could be found on the exact stoichiometry or the kinetics of the steps. Table 2 shows the chemical equations that have been proposed for the project and the components of the reactor effluent were assumed to be the same as the results provided in US Patent 209,795[3] and US Patent 324,778[4].

Table 2. Reaction network and heat of reaction per mass of C2 or C3 hydrocarbon consumed. Note that the reactions in which ethane and propane are consumed are endothermic.

| **Reaction Number** | **Stoichiometric Reaction** | **$\Delta H_{rxn}$ BTU/lb of C2 or C3 consumed** |
|---|---|---|
| 1 | $C_2H_6 + H_2 \rightarrow 2CH_4$ | -3.81 |
| 2 | $C_2H_6 \rightarrow C_2H_4 + H_2$ | 8.04 |
| 3 | $3C_2H_6 \rightarrow 2C_3H_6 + 3H_2$ | 5.76 |
| 4 | $3C_2H_6 \rightarrow 2C_3H_8 + H_2$ | 0.905 |
| 5 | $3C_2H_6 \rightarrow C_6H_6 + 6H_2$ | 5.92 |
| 6 | $4C_2H_6 \rightarrow C_7H_8 + CH_4 + 6H_2$ | 4.60 |
| 7 | $4C_2H_6 \rightarrow C_8H_{10} + CH_4 + 7H_2$ | 4.61 |
| 8 | $5C_2H_6 \rightarrow C_9H_{12} + CH_4 + 7H_2$ | 7.56 |
| 9 | $C_2H_4 + 2H_2 \rightarrow 2CH_4$ | -13.3 |
| 10 | $3C_2H_4 \rightarrow 2C_3H_6$ | -2.56 |
| 11 | $3C_2H_4 + 2H_2 \rightarrow 2C_3H_8$ | -8.03 |
| 12 | $3C_2H_4 \rightarrow C_6H_6 + 3H_2$ | -2.38 |
| 13 | $4C_2H_4 \rightarrow C_7H_8 + 2H_2 + CH_4$ | -3.87 |
| 14 | $4C_2H_4 \rightarrow C_8H_{10} + 3H_2$ | -3.86 |
| 15 | $4C_2H_4 \rightarrow C_9H_{12} + 2H_2 + CH_4$ | -0.543 |
| 16 | $2C_3H_8 \rightarrow C_6H_6 + 5H_2$ | 3.08 |
| 17 | $3C_3H_8 \rightarrow C_7H_8 + C_2H_6 + 5H_2$ | 2.21 |
| 18 | $3C_3H_8 \rightarrow C_8H_{10} + CH_4 + 5H_2$ | 1.70 |
| 19 | $3C_3H_8 \rightarrow C_9H_{12} + 3H_2$ | 4.86 |
| 20 | $C_3H_6 + H_2 \rightarrow CH_4 + C_2H_4$ | -1.07 |
| 21 | $2C_3H_6 \rightarrow C_6H_6 + 3H_2$ | 0.104 |
| 22 | $2C_3H_6 \rightarrow C_7H_8 + C_2H_6 + 2H_2$ | -0.803 |
| 23 | $3C_3H_6 \rightarrow C_8H_{10} + CH_4 + 2H_2$ | -1.34 |
| 24 | $3C_3H_6 \rightarrow C_9H_{12} + 6H_2$ | 1.97 |

Many of the reactions shown in Table 2 above are endothermic. Therefore the option of supplying heat to the reactor was considered when designing the reactor so that the reactants would remain at the reaction conditions of $1170^oF$.

# Process Charter

**Project Name:** BTX from Ethane

**Project Champion:** Richard Bockrath, Process Engineer - formerly DuPont
Daeyeon Lee, Associate Professor - University of Pennsylvania
Leonard Fabiano, Adjunct Professor - University of Pennsylvania

**Project Leaders:** Arthur Chen, Fiona Crowley, Jonathan Lym, Pablo Sanchez

**Specific Goals:** Design a preliminary competitive plant and process to create 0.5 million tons of BTX/year using fractional grade ethane.

**Project Scope:**

In Scope

- Fully specified equipment lists (sizing, materials, etc.) and subsequence process design
- Stoichiometric reactor model
- Catalyst specifications
- Methods of separation
- Size and configuration of recycle loops
- Cost analysis

Out of Scope

- Kinetic reactor model

**Deliverables:**

- Completed process model showing every piece of equipment and its specifications, including operating parameters.
- Capital cost and financial economic analyses demonstrating feasibility and profitability of the design.
- Written report describing our findings/design.
- PowerPoint presentation of our findings/design.

**Timeline:**

- Weekly progress reports until final report submitted.
- Written design report completed by Tuesday, April 14, 2015.
- Oral presentation given on Tuesday, April 21, 2015.

# Innovation Map

Recent breakthroughs in technology have made this process attractive. The innovation map, shown in Figure 2, shows how certain technologies affect the process and benefits customers.

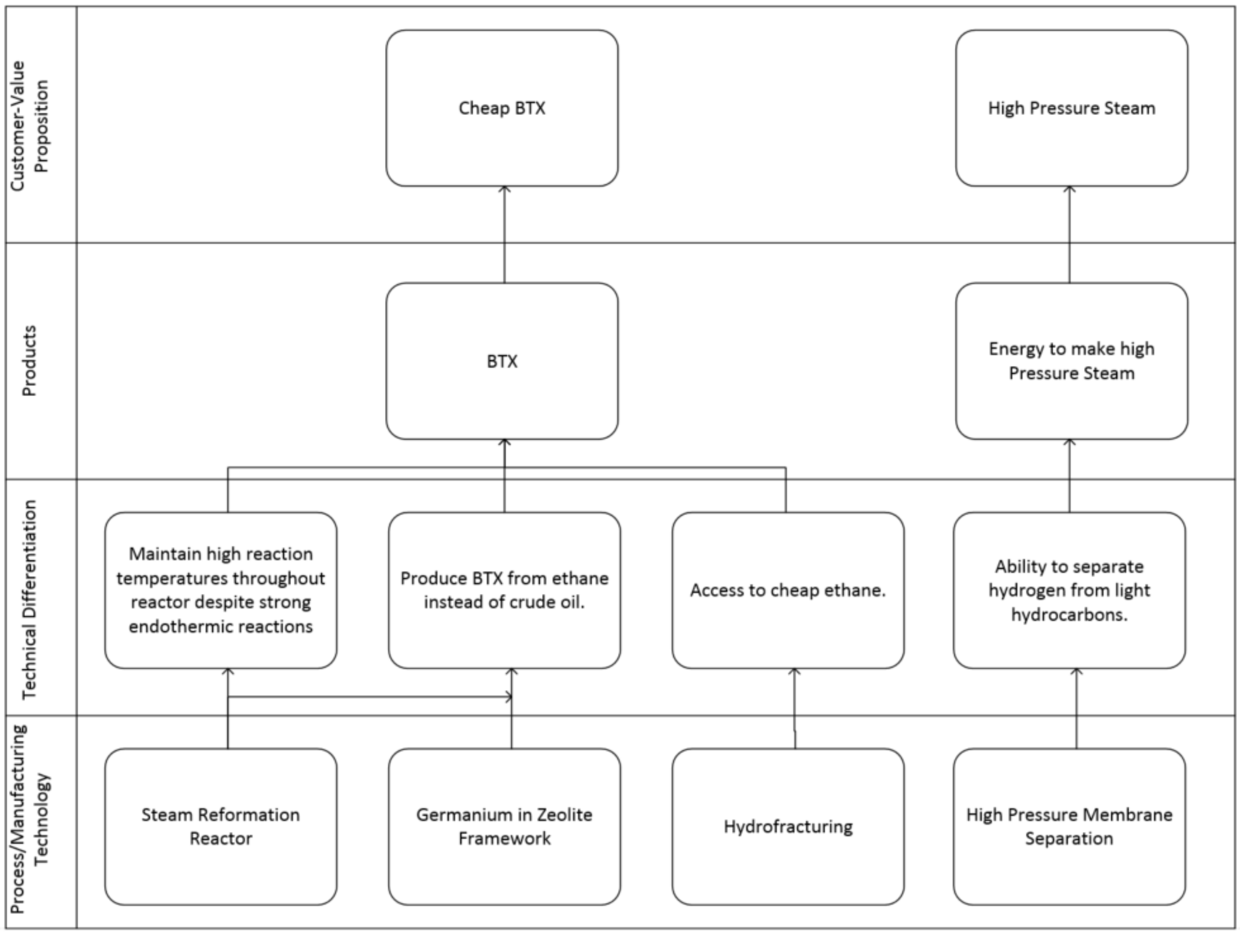


Figure 2. Innovation Map for the Proposed Process Design.

# Market and Competitive Analyses

## Market Analysis

### *The Use of Ethane over Oil*

Currently, BTX is primarily produced in plants using the method of naphthalene reformation from crude oil. As demand for crude oil inevitably increases in the near future, alternatives to the use of crude oil have been a major area of research due to the possibility of permanent increases in price over time. Besides economic reasons, the use of crude oil in general has become increasingly unpopular in recent years due to stigma regarding its importation from foreign sources and negative environmental impact. Due to the emergence of the hydraulic fracturing process to economically retrieve previously unreachable natural gas in shale rocks, the price of United States natural gas has fallen by 80% in the past five years from a 2008 price of about $10 per 1000 cubic feet to a current price of between $2 and $3 per 1000 cubic feet[5]. This low in the price of natural gas has opened an entirely new area of research into new uses of natural gas that could not have been considered earlier due to pricing issues. The study of the feasibility of producing BTX from natural gas components has been motivated by this price decrease, including a patent that converts propane to BTX. However, fractional grade ethane, which can be purchased as undesired byproduct from power plants, is substantially cheaper and readily available, and therefore worth studying as a feedstock for BTX production. For the purposes of this design project, the price of ethane is $0.067 per pound and is tabulated in Table 5.

Natural gas has traditionally been used as a source of energy and is currently the second largest energy source in the world behind crude oil. The use of natural gas for energy is preferred in our increasingly environmentally conscious world for reasons besides its economic benefits; its combustion releases 30% less carbon dioxide than oil and up to 45% less carbon dioxide than coal per Btu of heat produced. It is also in abundance in the U.S. as a domestic energy source with proven resources at 354 trillion cubic meters as of 2014, making up 5% of the world's proved reserves. Figure 5 shows the distribution of natural gas reserves by state in the United States.

The recent drop in crude oil prices is also a consideration, as this makes the traditional naphthalene reformation process of producing BTX more economically feasible. However, both natural gas and natural gas liquid (e.g. ethane) prices have dropped just as much, as seen in Figures 3 and 4. While the drop in crude oil prices has made some of the least profitable fracking companies stop drilling, the natural gas prices have not appeared to have been affected. If anything, natural gas prices have fallen alongside those of crude oil, making our process just as competitive as before the price drop.

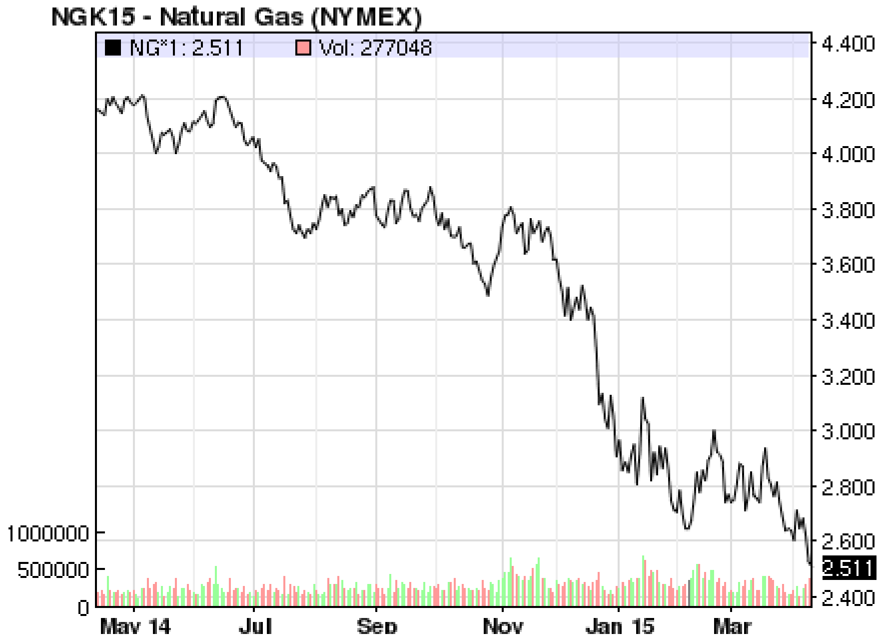


Figure 3. Natural gas prices from April 2014 to April 2015[5].


Figure 4. Ethane spot prices (per gallon) from December 2014 to April 2015[5].

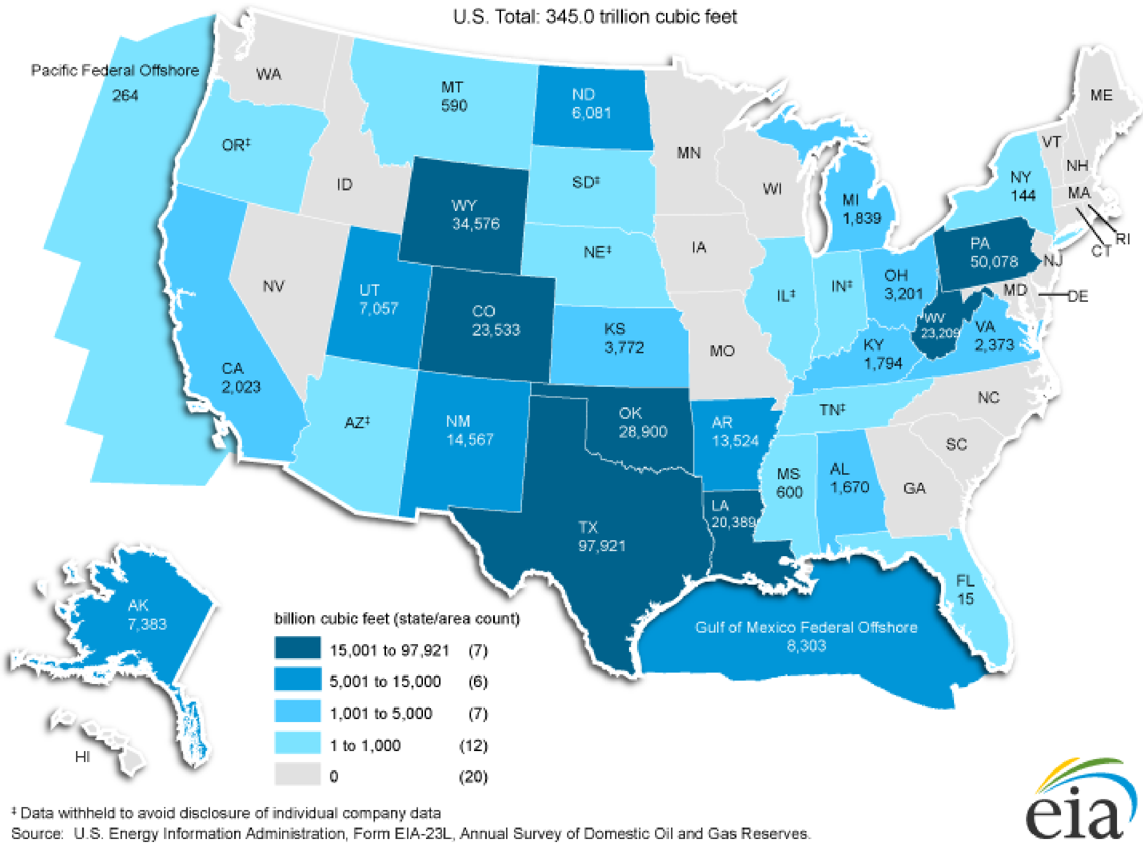


Figure 5. Natural gas proved reserves by sales/area, 2013[5]

*Benzene*

Benzene is the starting chemical reagent to create a wide array of aromatic chemical products. It is the most widely used aromatic petrochemical used in industrial processes. In the United States, about 50% of benzene is used to produce styrene, 20% is used to produce cumene, and 15% is used to produce nylon. Although the demand for benzene has been relatively stable in recent years, there are worries that weakening demand for polystyrene may negatively impact future prices of benzene. Despite this outlook, however, the price of benzene has been increasing in the past five years to a current high. For the purposes of this report, the price of our BTX mixture is taken to be $0.41 per pound as tabulated in Table 6.

*Toluene*

Toluene is a common organic solvent and is commonly used as paint thinner. The largest industrial use of toluene is in the production of benzene and xylene – making up over 46% of annual consumption in the United States. It is also used to make dyes, photographic chemicals, and pharmaceuticals. Its use is limited in consumer applications due to its status as a known carcinogen. The price of toluene is considered by the Independent Chemical Information Service as being volatile and is correlated to the price of gasoline. Because the majority of BTX produced is via crude oil cracking, as the price of crude oil has been increasing in the recent past, so has the price of toluene. It is predicted that production outages and political tensions are likely to keep the price of toluene volatile in the foreseeable future. For the purposes of this report, the price of our BTX mixture is taken to be $0.41 per pound as tabulated in Table 6.

*Xylene*

Para-xylene is the most valuable product per pound that is created in the production of BTX. It is used in the large scale to create the polyester PET, which is used to produce clothing fibers, plastic bottles, film, and other synthetic plastic and polymer products. The demand in the market for p-xylene is therefore highly correlated with the demand for PET polyesters and their derived products. Tecnon OrbiChem, a UK-based consulting firm, estimates world consumption to increase by 7% per year. This represents an attractive marketplace for new entrants such as our company. O-xylene is used in industry as a necessary agent to create plasticizers. The main application however for mixed xylenes is to be converted to more valuable p-xylene which can be then used for a wide variety of applications listed earlier. For the purposes of this report, the price of our BTX mixture is taken to be $0.41 per pound as tabulated in Table 6.

*BTX Market*

The market for BTX is currently valued at $80.8 billion in sales per year. According to IBISWorld reports, the market for BTX production is mature and very heavily regulated[26]. Although the industry is profitable and expected to grow at an average rate of 2.7% over the next four years to $96.2 billion in 2018, performance is heavily influenced by high levels of volatility. This level of growth is expected to be fuelled by the growth of the chemical and plastic product manufacturing industry. For example, the demand for housing starts which increase the demand for insulation derived from para-xylene is expected to grow at an annualized rate of 11.1%. The market for BTX is considered at this point to be mature due to product saturation and market acceptance. It is also outlined by clearly defined and segmented product groups and user industries as outlined in an industry report conducted by IBISWorld US in 2012. It is still possibly an attractive industry to enter, however, because of an expected shortage in supply to match the increase in demand expected through 2020. The primary markets are those in the domestic chemical manufacturing industry – only 1.8% of revenue of 2015 is predicted to be due to exports.

## Competitive Analysis

Competition in this market is seen to be medium but increasing due to the growth rate of the BTX industry and the potential for innovative methods of its production. The two largest competitors in this industry are Exxon Mobil Corporation and The Dow Chemical Company. Anellotech Inc. is another smaller competitor that aims to produce BTX products from renewable sources.

1. Exxon Mobil Chemical: Exxon Mobil Chemical is the petrochemical arm of Exxon Mobil Corporation. Exxon is one of the world's largest petrochemical companies. It is the largest North American producer of benzene and toluene and the second-largest producer of mixed xylene – holding an overall market share of 3.0%. Exxon, the country's largest oil refiner, is currently expanding their Texas facilities to take advantage of the close proximity to the gulf as well as further integrate the petroleum and petrochemical refining process. Its sales are estimated at $2.45 billion per year and it is expected to grow at an annual rate of 15.8%.

2. The Dow Chemical Company: Dow produces more than 5000 products in 197 manufacturing facilities in 36 countries. It is one of the largest petrochemical companies in the world. Unlike Exxon, Dow has its materials transferred to its chemical plants at a net cost. Dow currently operates six business segments with feedstocks and energy being the only relevant business segment to the petrochemical industry. In the five years to 2015, IBISWorld estimates that Dow's industry-specific revenue has increased at an annualized rate of 10.3% to $4.4 billion. It holds an overall BTX market share of 2.6%. Its sales are estimated at $2.1 billion per year.

3. Anellotech Inc.: Anellotech has developed a clean technology platform to inexpensively produce BTX from renewable biomass. It is expected that their products will be inexpensive compared to petroleum derived counterparts while providing identical benefit. Anellotech will own and operate its own plants and sell proprietary technology to licensees.

### *Porter's Five Forces*

The Porter's Five Forces framework is widely used in industry to identify and evaluate the competitive forces that must be considered when entering a prospective market. It was formed by Michael Porter of the Harvard Business School in 1979 as a tool to derive five market forces that determine the competitive industry and therefore the potential for profitability in a target market. The five forces are the (1) competitive rivalry within an industry, (2) bargaining power of suppliers, (3) bargaining power of customers, (4) threat of new entrants, and (5) threat of substitute products. By carefully considering how each of these forces affects our position in our target market, a more informed decision to enter the market can be made.

1. Competitive Rivalry Within the Industry

Currently, BTX is produced mostly via plants that incorporate naphthalene reforming processes from crude oil. The potential for new innovative processes to maintain a competitive advantage is inherently low as there are relatively few sources that hydrocarbons can be economically derived from sources other than fossil fuels. According to ICIS, some markets may be saturated in terms of the amount of BTX that is floating. In Asia, for example, there is an excess of benzene that is causing a cut in production to avoid a drop in price. Because existing BTX producers are dependent on the price of crude oil in order to justify the profitability of their operations, there is clearly a market opportunity in presenting an alternative and possibly more economical reagent such as natural gas. Because there are so many large competitors in the BTX production industry, however, competitive rivalry is expected to be high.

2. Bargaining Power of Suppliers

Because the natural gas that is needed for our process is plentiful in the Gulf Coast region, it is unlikely that suppliers will be able to pose a significant threat to our industry. This is because the infrastructure needed in the transportation of natural gas offsite is very expensive and the price of natural gas is determined largely by market forces. It would be relatively easy to switch to another supplier since the costs of changing suppliers will be low due to the high concentration of refineries in the region. Other suppliers, such as that of electricity and catalyst components, may have more bargaining power based on their higher flexibility to cater to other customers.

Suppliers of proprietary equipment needed to carry through with this process design have significant bargaining power that must be accounted for in making our final economic decision. Proprietary equipment such as the PRISM separation unit that must be purchased from outside vendors incurs a significant cost due to their necessity in our systems.

3. Bargaining Power of Consumers

The main threat that players in the BTX production industry face is the possibility of backward integration by consumers which would cut demand from producers like our company. Just as Coca-Cola recently invested in renewable para-xylene for their bottles, other customers may be more inclined to backwards integrate if the price of their supplies reaches a critical threshold. Many of the products that are derived from BTX incorporate a large portion of their overall costs from the price of BTX and so customers will be very price sensitive. Our BTX is undifferentiated from that of other companies, which causes a threat to us in terms of switching to a competitor. However, since we are treating ourselves as our own customer for BTX, these concerns are alleviated.

4. Threat of New Entrants

As the price of crude oil continues to decrease, there will continue to be an increasing economic interest in creating a method of producing BTX from alternative sources. In 2011, the Coca-Cola Company has invested in Geno, Virent, and Avantium partnerships in an aim to produce para-xylene for its bottles in a completely renewable fashion. This investment represents the kind of vertical integration that is very threatening for competitive players in this industry especially considering the increasing price of all BTX products.

In addition, barriers to entry into the industry are high, and are expected to remain that way. This industry faces a number of barriers to entry, a major one being the level of capital required. The costs to construct a plant can range anywhere from a couple hundred million to billions of dollars. For example, Dow Chemical Co. is in the works of securing permits to construct a $1.7 billion plant in Freeport, TX. Aside from the costs of building a plant, regulatory costs are high as well. Because the industry deals with chemical waste and emissions, companies are subject to rules set by the Environmental Protection Agency. Moreover, given the heavy reliance on various feedstocks, such as natural gas liquids and petroleum, the ability to access a steady supply of competitively priced raw materials is essential. Many of the established players are part of integrated oil companies that operate in integrated oil refining and petrochemical complexes, a position that gives them a significant competitive edge over potential stand-alone newcomers. Significant competition also comes from imported products. Infrastructure in oil rich nations, such as Saudi Arabia, continues to satisfy a large portion of domestic demand.

5. Threat of Substitute Products

The use of BTX in the products outlined in the Market Analysis section largely does not face a threat by substitute products. Benzene in particular cannot easily be replaced in industrial processes because it is the simplest six membered aromatic substance and many chemical processes rely on it to form product. The demand for Toluene is more price-sensitive because its use as a solvent can be replaced with other products. Para-xylene yields the most threat of substitute products because its use in hard plastic containers (PET) is threatened by a push to produce more renewable hard plastics. It should be considered, however, that with the overall trend toward higher prices for BTX that there will be an economic incentive to find substitutes and so there will be an increased effort in this area.

# Preliminary Process Synthesis

## Location of Plant

The two major concerns when determining the location of the plant were availability of ethane feedstock and cost of transporting the final BTX product. Our company is both a producer and a consumer of BTX, with customers in the Gulf Coast, Rotterdam, and Shanghai. The final decision to place the plant on the Gulf Coast was made due to both the ease of access to fractional-grade ethane from the numerous fracking operations in the area and to the proximity of BTX consumers. The cost of shipping liquid BTX is far lower than that of shipping ethane gas; therefore, the product can also be shipped to customers farther afield more economically. Additionally, the Gulf Coast has conveniently located pipelines for some of the reagents used for the catalyst regeneration process (i.e. nitrogen gas, oxygen gas, hydrogen gas).

## Reactor Model

An initial choice between fixed or fluidized bed models was made by referring to US Patent 209,795[3], which described the catalyst used in this process. In their experiments, the authors used a fixed bed packed with extrudate pellets; this and the high price of designing and scaling up a fluidized bed reactor motivated the choice of a fixed bed.

Due to the high temperature and endothermic nature of the reaction, a series of packed bed reactors would not be an efficient model, as seven reactors would be required to limit the temperature drop in each to less than 100°F. Therefore, the steam reformer model was selected, in which the feed is passed through tubes packed with catalyst, with direct heating on the outside of the tubes to maintain the necessary heat.

## Catalyst Choice

The problem statement recommended two catalysts developed in US Patent 324,778[4], each composed of a zeolite with platinum deposited on its surface, one with germanium incorporated into the zeolite structure and the other with titanium. The titanium catalyst had a higher overall conversion of about 80%, but a lower selectivity to BTX of about 40%. The germanium catalyst, on the other hand, had an overall conversion of about 40% but selectivity to BTX of about 52%. The patent gave conversions and selectivities for the conversion of propane to BTX, but these values were assumed to be the same for ethane to BTX. However, another patent, US Patent 209,795[3], was found, with a germanium catalyst specifically for the conversion of an ethane feedstock to BTX. This patent provided a more detailed breakdown of product selectivities and had a higher overall conversion (46.6%) and selectivity for aromatics (67.68%). The higher selectivity for BTX and the more knowledge available made the germanium catalyst a more attractive choice for this process.

US Patent 209,795[3] gave selectivity and conversion information of many catalysts. The tables found in the patent have been reproduced below. Table 3 shows catalysts A through I, which have varying levels of platinum and tin. Table 4 shows catalysts J through N, which have varying levels of platinum and germanium. Catalyst L was chosen as it offered the best combination of high conversion, high selectivity of BTX and low selectivity of inert byproducts like methane and C9+ hydrocarbons. Note that the conversion to C4 and C5 hydrocarbons was so low that it was assumed to be negligible. A catalyst with germanium present also benefitted the project as US Patent 324,778[4] could be used to provide conversion and selectivity data for any recycled propane to the reactor.

Table 3. US Patent 290,795 Selectivity and Conversion Data of Catalysts A through I, which all have different levels of platinum and tin.

| **Catalyst** | **A** | **B** | **C** | **D** | **E** | **F** | **G** | **H** | **I** |
|---|---|---|---|---|---|---|---|---|---|
| **Analyzed Pt Level, % wt.** | 0.006 | 0.011 | 0.025 | 0.0437 | 0.04 | 0.1 | 0.103 | 0.123 | 0.233 |
| **Analyzed Sn Level, % wt.** | 0.005 | 0.01 | 0.012 | 0.0395 | 0.093 | 0.076 | 0.0601 | 0.11 | 0.217 |
| **Ethane Conversion, %** | 44.4 | 44.72 | 48.02 | 50.39 | 45.42 | 55.44 | 61.62 | 55.73 | 56.6 |
| **Selectivities % (C basis)** | | | | | | | | | |
| **Methane** | 15.68 | 18.84 | 24.22 | 24.62 | 21.1 | 30.16 | 38.39 | 29.85 | 29.67 |
| **Ethylene** | 13.86 | 14.18 | 12.6 | 11.17 | 9.84 | 10.37 | 8.88 | 9.46 | 9.3 |
| **Propylene** | 2.23 | 2.13 | 1.63 | 1.36 | 1.27 | 1.1 | 0.85 | 0.97 | 0.86 |
| **Propane** | 1.67 | 1.69 | 1.4 | 1.23 | 1.56 | 0.91 | 0.64 | 0.84 | 0.76 |
| **C4 Hydrocarbons** | 0.46 | 0.43 | 0.33 | 0.28 | 0.28 | 0.24 | 0.18 | 0.21 | 0.19 |
| **C5 Hydrocarbons** | 0.04 | 0.04 | 0.01 | 0 | 0.01 | 0 | 0.01 | 0.01 | 0.04 |
| **Benzene** | 35.19 | 37.18 | 36.61 | 34.32 | 36.54 | 31.67 | 30.39 | 31.59 | 31.69 |
| **Toluene** | 18.48 | 19.28 | 18.27 | 18.05 | 19.17 | 16.34 | 14.85 | 16.53 | 15.94 |
| **C8 Aromatics** | 3.73 | 3.83 | 3.27 | 3.7 | 3.82 | 2.9 | 2.57 | 3.3 | 3 |
| **C9+ Aromatics** | 8.68 | 2.4 | 1.65 | 5.24 | 6.41 | 6.31 | 3.24 | 7.24 | 8.56 |
| **Total Aromatics** | 66.07 | 62.69 | 59.81 | 61.31 | 65.94 | 57.22 | 51.05 | 58.66 | 59.16 |
| **Total Desired Aromatics** | 57.4 | 60.29 | 58.15 | 56.07 | 59.53 | 50.91 | 47.81 | 51.42 | 50.63 |

Table 4. US Patent 290,795 Selectivity and Conversion Data of Catalysts J through N, which all have different levels of platinum and germanium. Note that the selected choice has been highlighted in gray.

| **Catalyst** | **J** | **K** | **L** | **M** | **N** |
|---|---|---|---|---|---|
| **Analyzed Pt Level, % wt.** | 0.046 | 0.0436 | 0.0441 | 0.0436 | 0.122 |
| **Analyzed Ge Level, % wt.** | 0.0216 | 0.0442 | 0.0844 | 0.121 | 0.1235 |
| **Ethane Conversion, %** | 46.94 | 46.39 | 46.6 | 45.07 | 50.16 |
| **Selectivities % (C basis)** | | | | | |
| **Methane** | 22.65 | 18.24 | 16.27 | 15.36 | 20.81 |
| **Ethylene** | 9.51 | 11.97 | 12.67 | 12.96 | 11.33 |
| **Propylene** | 1.19 | 1.5 | 1.54 | 1.65 | 1.2 |
| **Propane** | 1.44 | 1.48 | 1.47 | 1.62 | 1.15 |
| **C4 Hydrocarbons** | 0.27 | 0.32 | 0.34 | 0.36 | 0.29 |
| **C5 Hydrocarbons** | 0.03 | 0 | 0.04 | 0.02 | 0.03 |
| **Benzene** | 35.52 | 37.4 | 37.28 | 36.68 | 35.43 |
| **Toluene** | 19.25 | 19.8 | 19.85 | 19.73 | 18.35 |
| **C8 Aromatics** | 4.07 | 3.68 | 4.15 | 3.95 | 3.7 |
| **C9+ Aromatics** | 6.06 | 5.6 | 6.4 | 7.67 | 7.71 |
| **Total Aromatics** | 64.91 | 66.48 | 67.68 | 68.03 | 65.2 |
| **Total Desired Aromatics** | 58.84 | 60.88 | 61.28 | 60.36 | 57.48 |

## Catalyst Regeneration

The regeneration process was modeled after that given in US Patent 154,079[6], which laid out a five-step regeneration process for catalyst similar to that used in this process. It suggested a possible sixth step, in which the catalyst was sulfided. Sulfidation is used in regeneration processes to minimize coking, as sulfides break down groups of platinum on the surface of the catalyst into smaller ensembles, making it more difficult for coke to form. However, the sulfidation step was rejected due to the already lengthy nature of the regeneration process (the estimate used in this analysis was five and a half days) and to the potential poisoning of the catalyst.

## Separation of Hydrogen and Methane

Hydrogen and methane are produced in the reactors (see Figure 7) and have a detrimental effect on the equipment. The equipment that process hydrogen and methane had to be scaled larger to accommodate these species. Also, the separation of these components was necessary before using distillation columns as these species reduced the saturation temperature and increased the saturation pressure greatly. As a result, these components had to be removed.

The PRISM unit (see Figure 8) in the process is used to separate hydrogen and methane. However, a pressure-swing adsorption system was considered for the process as well. The PRISM system was preferred as it was difficult to find a suitable surface that would be able to bind all the other components of the stream. Additional costs would arise in order to refrigerate the system to temperatures to desorb its contents. Also, a pressure-swing adsorption system would complicate the process as the batch nature of the adsorption and desorption process will have to be managed.

## Purge

The most expensive pieces of equipment in the process are the compressors (see Figure 8) valued at $18,221,847 each; the reactors (see Figure 7) valued at $55,000,000; and the PRISM Separation Unit (see Figure 8) valued at $17,000,000. These units are so expensive due to the large flow rates around the process. The flows could be reduced by implementing a purge stream. Stream S-211 (see Figure 8) is the optimal candidate to purge as it contains no BTX product. If this stream were purged and its contents burned, more high-pressure steam could be generated and sold and the size and, as a result, the cost of several pieces of equipment could be reduced due to the lower demand on the units (heat exchangers H-201, H-202, and H-203, PRISM unit PR-101, turbines T-101, T-102, and T-103, reactor R-101, R-102, R-103, compressors C-201 and C-202). On the other hand, more fractional grade ethane would have to be obtained as some of the purged stream contains valuable reactants that could have been recycled into the reactor; the cost of the steam boilers would have to be adjusted to accommodate the larger heat duty; and the turbines in Section 1 (see Figure 7) would produce less electricity. Unfortunately, the purge option could not be investigated in full detail as estimates for the costs of the PRISM unit and the reactors with the adjusted flow rates could not be obtained. However, it remains an option for potential future study if this project is taken into further development.

## Lifetime of Catalyst

As testing of this catalyst has only occurred at a lab scale and information on its lifespan was not provided in the patent, an assumption of catalyst lifetime had to be made. Of catalytic processes commonly used, this is most similar to naphtha reform, which uses platinum alloys supported on alumina[7]. This process occurs at harsh operating conditions, with temperatures ranging from 860 to 980°F and pressures of 120 to 740 psi. Catalysts can last up to six months; therefore, a lifespan of one month was used as a conservative assumption for the germanium-incorporated zeolites used in this process.

# Assembly of Database

## Thermodynamic and Transport Data

All transport and thermodynamic data were taken from the ASPEN Plus Program and used directly in models. The Redlich-Kwong equation of state was the thermodynamic model used for gaseous species and the NRTL equation of state was used for liquid species.

## Pricing Data

The prices for the inputs and outputs of the process were compiled from various sources.

### *Feed Materials*

Table 5: Mass flow rate and price for feed materials.[8-13]

| **Material Name** | **Mass Flow Rate (lb/year)** | **Price ($/lb)** |
|---|---|---|
| Fractional Grade Ethane | 1.47E+09 | 0.067 |
| Chlorine | 1.07E+07 | 0.68 |
| Oxygen | 4.12E+07 | 0.09 |
| Hydrogen | 6.78E+06 | 0.64 |
| Nitrogen | 3.39E+08 | 0.18 |

### *Products*

Table 6: Mass flow rate, density and price for products of the process.[14,15]

| **Product Name** | **Mass Flow Rate (lb/year)** | **Density (lb/gal)** | **Price ($/gal)** | **Price ($/1000 lb)** |
|---|---|---|---|---|
| BTX | 9.04E+08 | 7.26 | 3.0 | - |
| Gasoline Blend | 9.26E+07 | 7.31 | 3.0 | - |
| High Pressure Steam (450 psig) | 8.06E+09 | - | - | 8.0 |

*Catalyst*

Table 7: Mass required per year and the price of the catalyst components. Note that this mass assumes that catalyst has to be purchased every month.[16-18]

| Catalyst Component | Mass Required (lb/year) | Price ($/lb) |
|---|---|---|
| Germanium | 59840 | 862 |
| Platinum | 31210 | 18240 |
| Zeolite | 5.66E+07 | 5.67 |
| Alumina | 1.42E+07 | 0.159 |

*Utilities*

Table 8: Amount of each utility used and the corresponding price.[14]

| Utility | Amount Required (Unit/year) | Price ($/Unit) |
|---|---|---|
| Cooling Water | 3.20E+10 lb | 0.0120/1000 lb |
| Process Water | 8.06E+09 lb | 0.0962/1000 lb |
| Electricity | 2.59E+08 kWh | 0.07/kWh |

## Safety and MSDS

The Material Safety Data Sheets for the chemicals used in this process are provided in Appendix A-4: Thermophysical Data & Material Safety Data Sheets for reference.

# Process Flowsheet and Material Balances

For the ease of reading, the following process is divided into four connected sections. An overview has been provided in Figure 6. A description of the process may be found under the Process Description Section. The process flow diagram will be presented on the left and mass flow of each material, temperature, pressure, vapor/liquid fraction, and enthalpy is shown on the following pages.

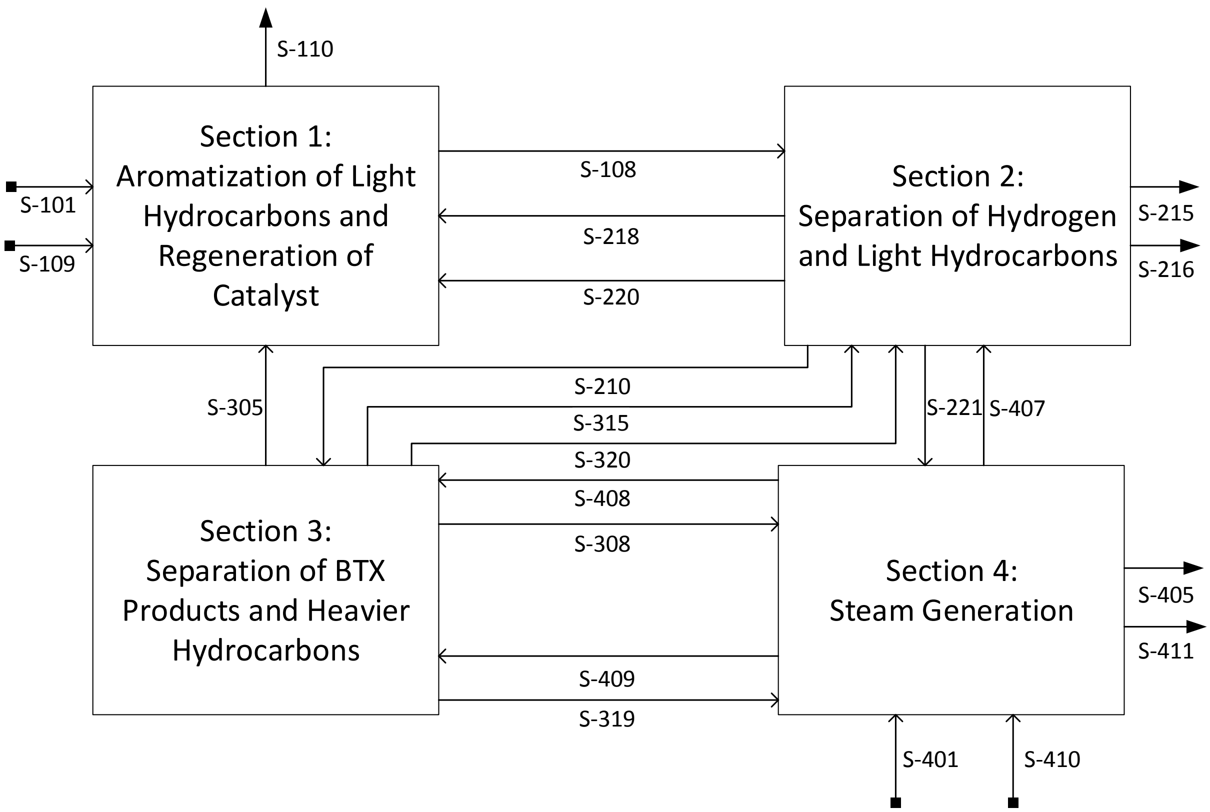


Figure 6. Overview of the interactions among the four different sections of the process.

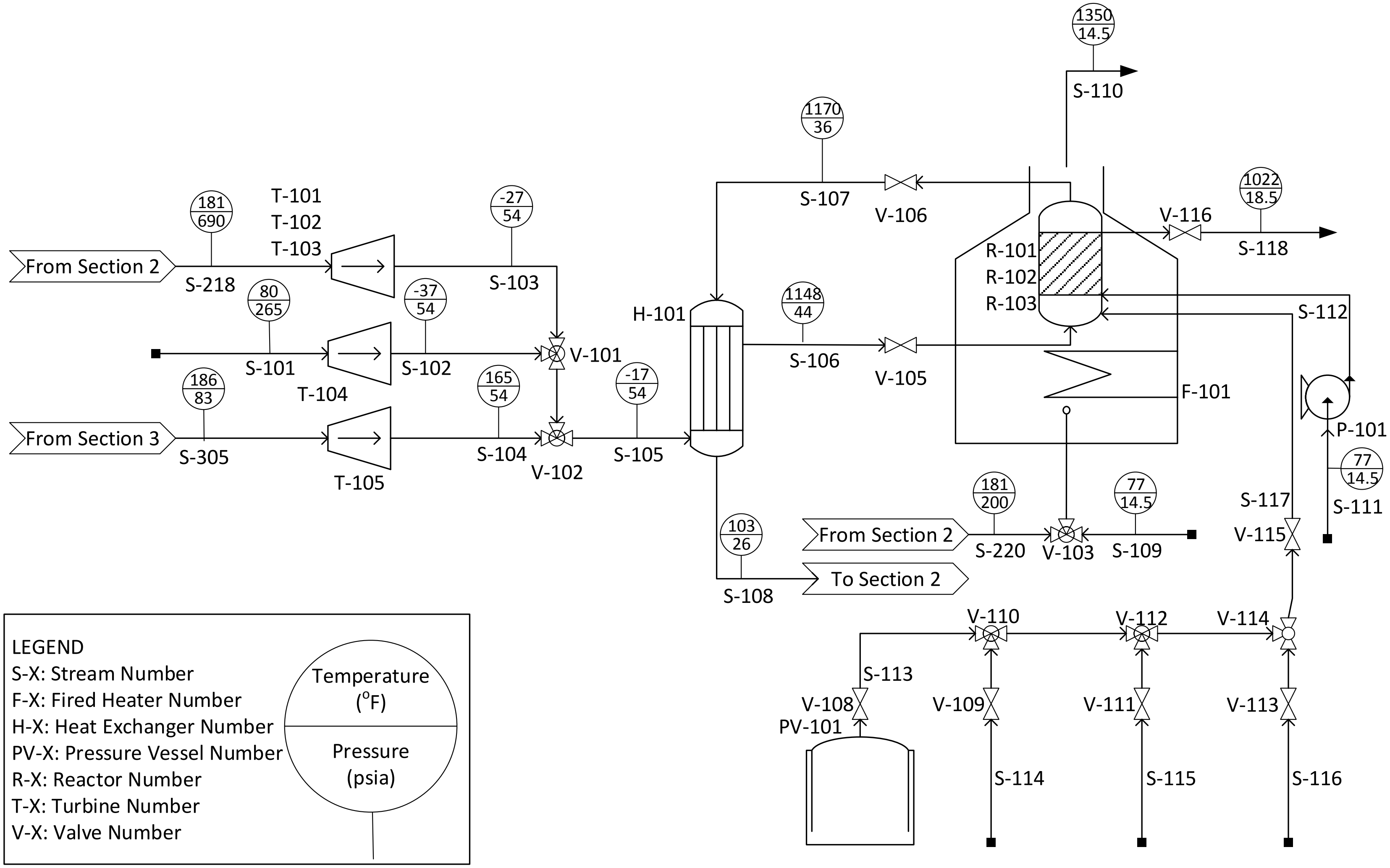


Figure 7. Section 1: Aromatization of Light Hydrocarbons and Regeneration of Catalyst

Table 9. Stream Report of Streams S-101 to S-110 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| | **Mass Flow (lb/hr)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-101 | S-102 | S-103 | S-104 | S-105 | S-106 | S-107 | S-108 | S-109 | S-110 |
| Hydrogen | 0 | 0 | 2758 | Trace | 2758 | 2758 | 18388 | 18388 | 0 | 0 |
| Methane | 989 | 989 | 115104 | 2717 | 118810 | 118810 | 162584 | 162584 | 0 | 0 |
| Ethane | 179794 | 179794 | 202499 | 7038 | 389331 | 389331 | 209537 | 209537 | 0 | 0 |
| Ethylene | 0 | 0 | 21482 | 608 | 22090 | 22090 | 22090 | 22090 | 0 | 0 |
| Propane | 5436 | 5436 | 8316 | 711 | 14463 | 14463 | 9027 | 9027 | 0 | 0 |
| Propylene | 0 | 0 | 2630 | 143 | 2774 | 2774 | 2774 | 2774 | 0 | 0 |
| Benzene | 0 | 0 | 9641 | 8373 | 18014 | 18014 | 88283 | 88283 | 0 | 0 |
| Toluene | 0 | 0 | 397 | 835 | 1232 | 1232 | 35905 | 35905 | 0 | 0 |
| P-Xylene | 0 | 0 | 3.73 | 23.7 | 27.5 | 27.5 | 9178 | 9178 | 0 | 0 |
| 1,3,5-Trimethyl Benzene | 0 | 0 | Trace | Trace | Trace | Trace | 11739 | 11739 | 0 | 0 |
| Water | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 42201 |
| Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 63797 | 10633 |
| Nitrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 210109 | 210109 |
| Carbon Dioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 21573 |
| Total Flow (lb/hr) | 186219 | 186219 | 362832 | 20449 | 569500 | 569500 | 569504 | 569504 | 273906 | 284516 |
| Total Flow (cuft/hr) | 114604 | 490675 | 1371780 | 67664 | 1960370 | 9149310 | 13895200 | 6551820 | 3768190 | 14251200 |
| Temperature ($^{o}$F) | 80.0 | -37 | -27 | 165 | -17 | 1148 | 1166 | 103 | 77.0 | 1346 |
| Pressure (psia) | 265 | 53.7 | 53.7 | 53.7 | 53.7 | 43.7 | 36.4 | 26.4 | 14.5 | 14.5 |
| Vapor Frac | 1.00 | 1.00 | 0.99 | 0.99 | 0.99 | 1.00 | 1.00 | 0.99 | 1.00 | 1.00 |
| Liquid Frac | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 | 0.00 | 0.00 | 0.01 | 0.00 | 0.00 |
| Enthalpy (Btu/lb) | -1.21E+3 | -1.25E+3 | -1.32E+3 | -4.65E+2 | -1.26E+3 | -4.55E+2 | -9.35E+1 | -9.03E+2 | -1.00E-1 | -7.74E+2 |
| Enthalpy (Btu/hr) | -2.26E+8 | -2.32E+8 | -4.79E+8 | -9.50E+6 | -7.20E+8 | -2.59E+8 | -5.33E+7 | -5.14E+8 | -2.74E+4 | -2.20E+8 |

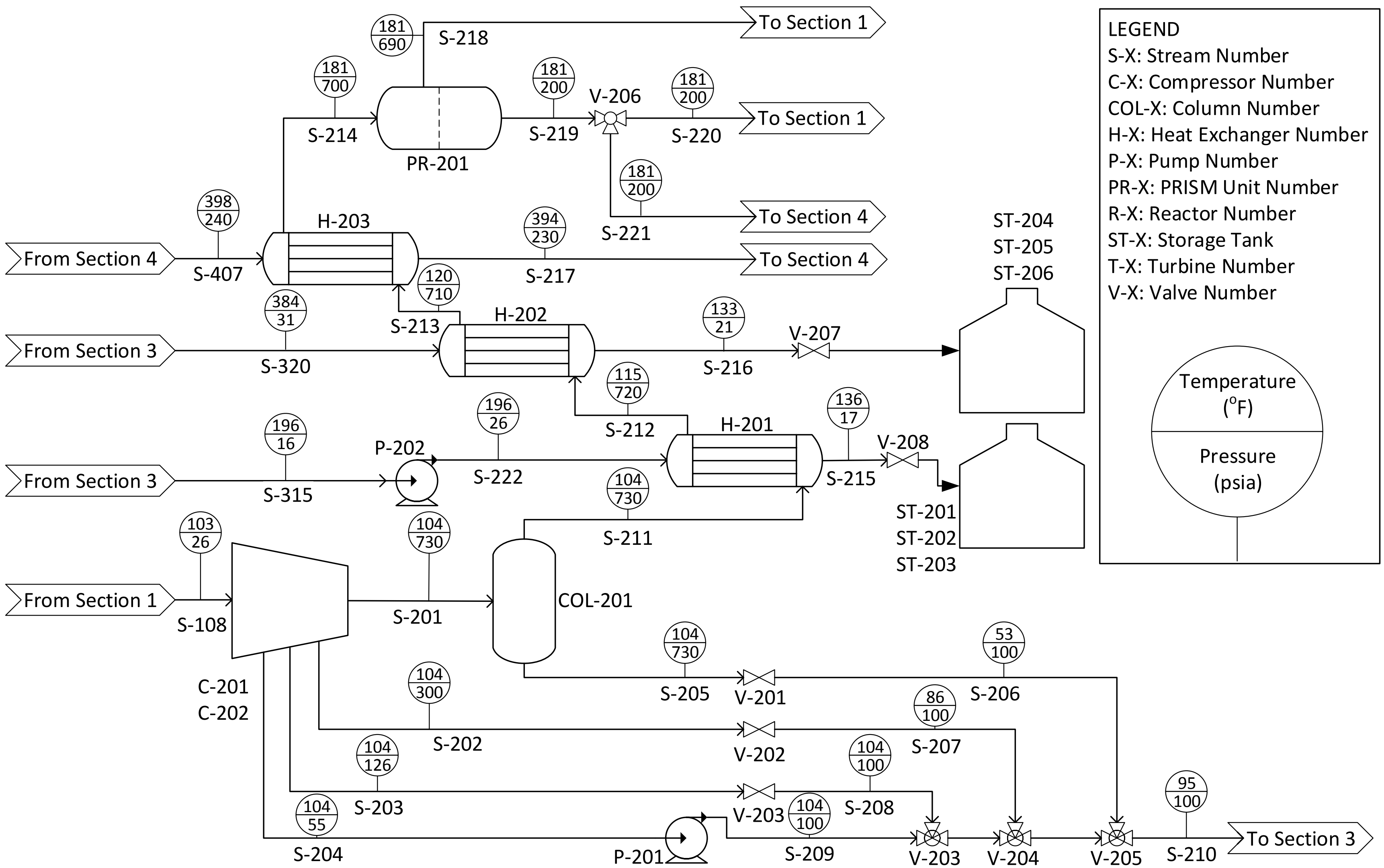


Figure 8. Section 2: Separation of Hydrogen and Light Hydrocarbons

Table 10. Stream Report of Streams S-201 to S-210 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| | **Mass Flow (lb/hr)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-201 | S-202 | S-203 | S-204 | S-205 | S-206 | S-207 | S-208 | S-209 | S-210 |
| Hydrogen | 18388 | Trace | Trace | Trace | Trace | Trace | Trace | Trace | Trace | Trace |
| Methane | 161167 | 783 | 391 | 243 | 1301 | 1301 | 783 | 391 | 243 | 2717 |
| Ethane | 205548 | 2131 | 1135 | 723 | 3049 | 3049 | 2131 | 1135 | 723 | 7038 |
| Ethylene | 21752 | 182 | 95.5 | 60.5 | 270 | 270 | 182 | 95.5 | 60.5 | 608 |
| Propane | 8615 | 217 | 119 | 76.5 | 298 | 298 | 217 | 119 | 76.5 | 711 |
| Propylene | 2695 | 40.9 | 22.2 | 15.7 | 64.2 | 64.2 | 40.9 | 22.2 | 15.7 | 143 |
| Benzene | 20942 | 20551 | 23052 | 23738 | 11301 | 11301 | 20551 | 23052 | 23738 | 78642 |
| Toluene | 1654 | 4717 | 10593 | 18941 | 1257 | 1257 | 4717 | 10593 | 18941 | 35508 |
| P-Xylene | 35.4 | 300 | 1726 | 7117 | 31.6 | 31.6 | 300 | 1726 | 7117 | 9175 |
| 1,3,5-Trimethyl Benzene | 2.56 | 61.2 | 967 | 10708 | 2.45 | 2.45 | 61.2 | 967 | 10708 | 11739 |
| Total Flow (lb/hr) | 440798 | 28984 | 38100 | 61622 | 17574 | 17574 | 28984 | 38100 | 61622 | 146280 |
| Total Flow (cuft/hr) | 210921 | 617 | 755 | 1191 | 448 | 8454 | 4019 | 755 | 1191 | 9756 |
| Temperature ($^oF$) | 104 | 104 | 104 | 104 | 104 | 53.2 | 86.3 | 104 | 104 | 96.0 |
| Pressure (psia) | 730 | 300 | 126 | 55.1 | 730 | 100 | 100 | 100 | 100 | 100 |
| Vapor Frac | 0.99 | 0.00 | 0.00 | 0.00 | 0.00 | 0.43 | 0.14 | 0.00 | 0.00 | 0.06 |
| Liquid Frac | 0.01 | 1.00 | 1.00 | 1.00 | 1.00 | 0.57 | 0.86 | 1.00 | 1.00 | 0.94 |
| Enthalpy (Btu/lb) | -1.25E+3 | 5.26E+1 | 1.17E+2 | 5.66E+1 | -2.04E+2 | -2.04E+2 | 5.26E+1 | 1.17E+2 | 5.68E+1 | 4.03E+1 |
| Enthalpy (Btu/hr) | -5.53E+8 | 1.53E+6 | 4.45E+6 | 3.49E+6 | -3.59E+6 | -3.59E+6 | 1.53E+6 | 4.45E+6 | 3.50E+6 | 5.89E+6 |

Table 11. Stream Report of Streams S-211 to S-220 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| | **Mass Flow (lb/hr)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-211 | S-212 | S-213 | S-214 | S-215 | S-216 | S-217 | S-218 | S-219 | S-220 |
| Hydrogen | 18388 | 18388 | 18388 | 18388 | 0 | 0 | 0 | 2758 | 15630 | 2746 |
| Methane | 159866 | 159866 | 159866 | 159866 | 0 | 0 | 0 | 115104 | 44762 | 7864 |
| Ethane | 202499 | 202499 | 202499 | 202499 | 0 | 0 | 0 | 202499 | 0 | 0 |
| Ethylene | 21482 | 21482 | 21482 | 21482 | 0 | 0 | 0 | 21482 | 0 | 0 |
| Propane | 8316 | 8316 | 8316 | 8316 | 0 | 0 | 0 | 8316 | 0 | 0 |
| Propylene | 2630 | 2630 | 2630 | 2630 | 0 | 0 | 0 | 2630 | 0 | 0 |
| Benzene | 9641 | 9641 | 9641 | 9641 | 70269 | Trace | 0 | 9641 | 0 | 0 |
| Toluene | 397 | 397 | 397 | 397 | 34673 | Trace | 0 | 397 | 0 | 0 |
| P-Xylene | 3.73 | 3.73 | 3.73 | 3.73 | 9136 | 14.7 | 0 | 3.73 | 0 | 0 |
| 1,3,5-Trimethyl Benzene | Trace | Trace | Trace | Trace | 40.5 | 11698 | 0 | Trace | 0 | 0 |
| Water | 0 | 0 | 0 | 0 | 0 | 0 | 22826 | 0 | 0 | 0 |
| Total Flow (lb/hr) | 423224 | 423224 | 423224 | 423224 | 114118 | 11713 | 22826 | 362832 | 60392 | 10610 |
| Total Flow (cuft/hr) | 210472 | 218944 | 224528 | 256757 | 2192 | 224 | 3033 | 147963 | 364193 | 63983 |
| Temperature ($^oF$) | 104 | 115 | 120 | 181 | 136 | 133 | 394 | 181 | 181 | 181 |
| Pressure (psia) | 730 | 720 | 710 | 700 | 16.0 | 22.0 | 230 | 690 | 200 | 200 |
| Vapor Frac | 1.00 | 1.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.05 | 1.00 | 1.00 | 1.00 |
| Liquid Frac | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 1.00 | 0.95 | 0.00 | 0.00 | 0.00 |
| Enthalpy (Btu/lb) | -1.30E+3 | -1.29E+3 | -1.29E+3 | -1.24E+3 | 2.01E+2 | -2.03E+2 | -6.43E+3 | -1.23E+3 | -1.35E+3 | -1.35E+3 |
| Enthalpy (Btu/hr) | -5.49E+8 | -5.46E+8 | -5.44E+8 | -5.27E+8 | 2.29E+7 | -2.37E+6 | -1.47E+8 | -4.47E+8 | -8.13E+7 | -1.43E+7 |

Table 12. Stream Report of Streams S-221 to S-222 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| **Species** | **Mass Flow (lb/hr)** | |
|---|---|---|
| | S-221 | S-222 |
| Hydrogen | 12884 | 0 |
| Methane | 36898 | 0 |
| Benzene | 0 | 70269 |
| Toluene | 0 | 34673 |
| P-Xylene | 0 | 9136 |
| 1,3,5-Trimethyl Benzene | 0 | 40.5 |
| Total Flow (lb/hr) | 49782 | 114118 |
| Total Flow (cuft/hr) | 300210 | 2287 |
| Temperature ($^oF$) | 181 | 196 |
| Pressure (psia) | 200 | 26.0 |
| Vapor Frac | 1.00 | 0.00 |
| Liquid Frac | 0.00 | 1.00 |
| Enthalpy (Btu/lb) | -1.35E+3 | 2.29E+2 |
| Enthalpy (Btu/hr) | -6.70E+7 | 2.62E+7 |

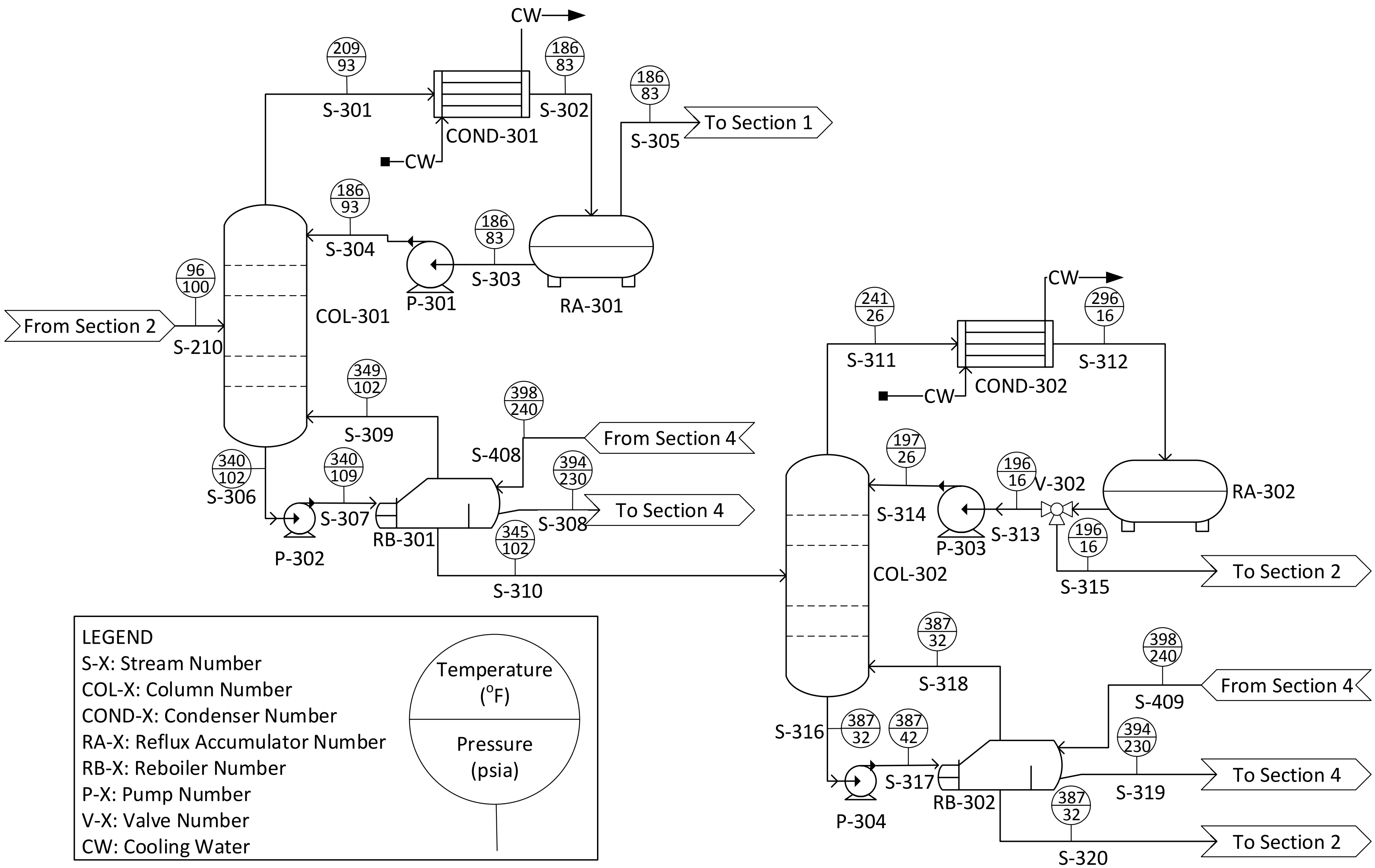


Figure 9. Section 3: Separation of BTX Products and Heavier Hydrocarbons

Table 13. Stream Report of Streams S-301 to S-310 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| | **Mass Flow (lb/hr)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-301 | S-302 | S-303 | S-304 | S-305 | S-306 | S-307 | S-308 | S-309 | S-310 |
| Hydrogen | Trace | Trace | Trace | Trace | Trace | Trace | Trace | 0 | Trace | Trace |
| Methane | 2723 | 2723 | 5.39 | 5.39 | 2717 | Trace | Trace | 0 | Trace | Trace |
| Ethane | 7089 | 7089 | 50.7 | 50.7 | 7038 | Trace | Trace | 0 | Trace | Trace |
| Ethylene | 612 | 612 | 3.61 | 3.61 | 608 | Trace | Trace | 0 | Trace | Trace |
| Propane | 720 | 720 | 9.08 | 9.08 | 711 | Trace | Trace | 0 | Trace | Trace |
| Propylene | 144 | 144 | 1.07 | 1.07 | 143 | Trace | Trace | 0 | Trace | Trace |
| Benzene | 10037 | 10037 | 1664 | 1664 | 8373 | 174298 | 174298 | 0 | 104030 | 70269 |
| Toluene | 1186 | 1186 | 351 | 351 | 835 | 61609 | 61609 | 0 | 26936 | 34673 |
| P-Xylene | 42.8 | 42.8 | 19.1 | 19.1 | 23.7 | 13244 | 13244 | 0 | 4094 | 9151 |
| 1,3,5-Trimethyl Benzene | Trace | Trace | Trace | Trace | Trace | 14893 | 14893 | 0 | 3154 | 11739 |
| Water | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25705 | 0 | 0 |
| Total Flow (lb/hr) | 22553 | 22553 | 2104 | 2104 | 20449 | 264044 | 264044 | 25705 | 138214 | 125831 |
| Total Flow (cuft/hr) | 43772 | 36943 | 43.2 | 43.2 | 45287 | 6005 | 6006 | 3187 | 3177 | 2883 |
| Temperature ($^oF$) | 209 | 186 | 186 | 186 | 186 | 340 | 340 | 394 | 349 | 349 |
| Pressure (psia) | 93.0 | 83.0 | 83.0 | 93.0 | 83.0 | 102 | 109 | 230 | 102 | 102 |
| Vapor Frac | 1.00 | 0.90 | 0.00 | 0.00 | 1.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.00 |
| Liquid Frac | 0.00 | 0.10 | 1.00 | 1.00 | 0.00 | 1.00 | 1.00 | 0.95 | 1.00 | 1.00 |
| Enthalpy (Btu/lb) | -3.65E+2 | -4.07E+2 | 2.30E+2 | 2.30E+2 | -4.53E+2 | 3.03E+2 | 3.03E+2 | -6.43E+3 | 3.40E+2 | 2.72E+2 |
| Enthalpy (Btu/hr) | -8.23E+6 | -9.18E+6 | 4.83E+5 | 4.83E+5 | -9.27E+6 | 7.99E+7 | 7.99E+7 | -1.65E+8 | 4.70E+7 | 3.42E+7 |

Table 14. Stream Report of Streams S-311 to S-320 showing the mass flow of each material, the temperature, pressure, vapor/liquid fraction and enthalpy.

| | **Mass Flow (lb/hr)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-311 | S-312 | S-313 | S-314 | S-315 | S-316 | S-317 | S-318 | S-319 | S-320 |
| Benzene | 115357 | 115357 | 70269 | 70269 | 70269 | Trace | Trace | Trace | 0 | Trace |
| Toluene | 56920 | 56920 | 34673 | 34673 | 34673 | Trace | Trace | Trace | 0 | Trace |
| P-Xylene | 14998 | 14998 | 9136 | 9136 | 9136 | 404 | 404 | 389 | 0 | 14.7 |
| 1,3,5-Trimethyl Benzene | 66.5 | 66.5 | 40.5 | 40.5 | 40.5 | 194050 | 194050 | 182351 | 0 | 11698 |
| Total Flow (lb/hr) | 187342 | 187342 | 114118 | 114118 | 114118 | 194453 | 194453 | 182741 | 31936 | 11713 |
| Total Flow (cuft/hr) | 620515 | 3755 | 2287 | 2287 | 2287 | 4449 | 4449 | 406501 | 4501 | 268 |
| Temperature ($^{o}$F) | 241 | 196 | 196 | 197 | 196 | 387 | 387 | 387 | 394 | 387 |
| Pressure (psia) | 26.0 | 16.0 | 16.0 | 45.0 | 16.0 | 31.9 | 41.9 | 32.0 | 230 | 32.0 |
| Vapor Frac | 1.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 0.06 | 0.00 |
| Liquid Frac | 0.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.00 | 0.94 | 1.00 |
| Enthalpy (Btu/lb) | 4.06E+2 | 2.29E+2 | 2.29E+2 | 2.29E+2 | 2.29E+2 | -7.64E+1 | -7.64E+1 | 5.56E+1 | -6.43E+3 | -7.63E+1 |
| Enthalpy (Btu/hr) | 7.60E+7 | 4.30E+7 | 2.62E+7 | 2.62E+7 | 2.62E+7 | -1.49E+7 | -1.49E+7 | 1.02E+7 | -2.05E+8 | -8.94E+5 |

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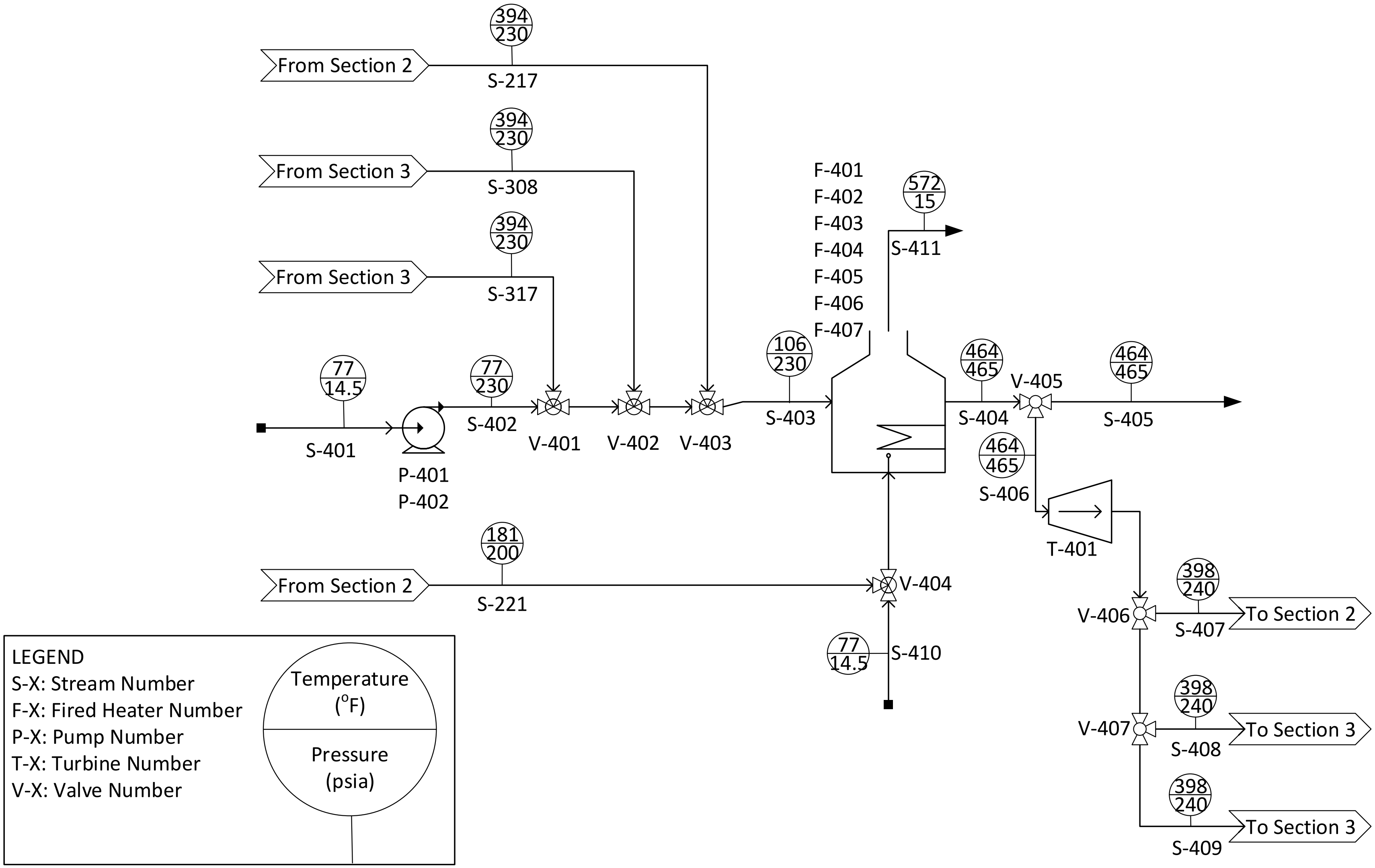

Figure 10. Section 4: Steam Generation

Table 15. Stream Report of Streams S-401 to S-410 showing the mass flow of each material, the temperature, pressure, vapour/liquid fraction and enthalpy.

| | Mass Flow (lb/hr) | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Species** | S-401 | S-402 | S-403 | S-404 | S-405 | S-406 | S-407 | S-408 | S-409 | S-410 |
| Water | 1015890 | 1015890 | 1096360 | 1096360 | 1015890 | 80467 | 22826 | 25705 | 31936 | 0 |
| Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 299340 |
| Nitrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 985838 |
| Total Flow (lb/hr) | 1015890 | 1015890 | 1096360 | 1096360 | 1015890 | 80467 | 22826 | 25705 | 31936 | 1285180 |
| Total Flow (cuft/hr) | 16372 | 16374 | 17955 | 1165440 | 1079910 | 85537 | 43974 | 49520 | 61524 | 17680500 |
| Temperature ($^oF$) | 77.0 | 77.2 | 106 | 465 | 465 | 465 | 398 | 398 | 398 | 77.0 |
| Pressure (psia) | 14.5 | 230 | 230 | 465 | 465 | 465 | 240 | 240 | 240 | 14.5 |
| Vapor Frac | 0.00 | 0.00 | 0.00 | 1.00 | 1.00 | 1.00 | 0.97 | 0.97 | 0.97 | 1.00 |
| Liquid Frac | 1.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.03 | 0.03 | 0.00 |
| Enthalpy (Btu/lb) | -6.82E+3 | -6.82E+3 | -6.79E+3 | -5.62E+3 | -5.62E+3 | -5.62E+3 | -5.67E+3 | -5.67E+3 | -5.67E+3 | -1.00E-1 |
| Enthalpy (Btu/hr) | -6.93E+9 | -6.93E+9 | -7.45E+9 | -6.17E+9 | -5.71E+9 | -4.52E+8 | -1.29E+8 | -1.46E+8 | -1.81E+8 | -1.29E+5 |

Table 16. Stream Report of Stream S-411 showing the mass flow of each material, the temperature, pressure, vapour/liquid fraction and enthalpy.

| | Mass Flow (lb/hr) |
|---|---|
| **Species** | S-411 |
| Water | 198009 |
| Oxygen | 49890 |
| Nitrogen | 985838 |
| Carbon Dioxide | 101223 |
| Total Flow (lb/hr) | 1334960 |
| Total Flow (cuft/hr) | 38194900 |
| Temperature ($^oF$) | 572 |
| Pressure (psia) | 14.5 |
| Vapor Frac | 1.00 |
| Liquid Frac | 0.00 |
| Enthalpy (Btu/lb) | -1.01E+3 |
| Enthalpy (Btu/hr) | -1.35E+9 |

# Process Description

## Section 1 - Aromatization of Light Hydrocarbons and Regeneration of Catalyst

Light hydrocarbons, such as ethane, ethylene, propane and propylene, in this section are reacted to form benzene, toluene and xylene.

### *Pretreatment*

Firstly, stream S-101, which contains fractional-grade ethane with a mole composition of 1% methane, 97% ethane and 2% propane[18], enters the process through available pipelines along the Gulf Coast at a temperature of 88$^{o}$F and a pressure of 265 psia. This feed stream will mix with S-218, the retentate of the PRISM system from Section 2, and S-305, the distillate of the Distillation Column COL-301 from Section 3. These streams contain mostly C2 and C3. The streams must be expanded to a suitable pressure to undergo aromatization. Each stream passes through a turbine that will reduce its pressure to 54 psia and produce some electricity. The streams mix and then are fed to the pretreatment section of the reactor, a heat exchanger that transfers heat between the inlet of the reactor and the outlet, H-101. The stream is preheated from -17$^{o}$F to 1148$^{o}$F.

### *Aromatization*

The preheated stream, S-106, then enters the furnace where it is heated to 1170$^{o}$F and then passes into one of the three reactors, R-101, R-102, and R-103. These reactors are steam-reforming type reactors, provided by the Jacobs Engineering Group, in which tubes packed with catalysts are enclosed in a furnace, are maintained at a temperature of 1170$^{o}$F by using fired heaters on the outsides of the tubes. This temperature is maintained by continuously burning hydrogen and methane recovered from the permeate of the PRISM separation unit in Section 2 with 20% excess air. The feed entered the reactor at a pressure of 43.7 psia and left at a pressure of 36.4 psia; these pressures were selected to permit flow through the packed tubes. It was assumed in this analysis that the conversions and selectivities given in the patents would remain the same at these higher pressures. The reactor effluent, S-107 contains a wide array of products, including methane, C2 and C3 alkanes and alkenes, benzene, toluene, xylene, and heavier hydrocarbons.

The selectivity and conversion of ethane was provided by US Patent 209,795[2] and the selectivity was assumed to be the same as ethane. However, since the conversion of ethane to ethylene was the rate-limiting step, it was assumed that all the ethylene entering the reactor would be consumed. The specific catalyst chosen and the corresponding conversion and selectivity are shown under the 'Catalyst Choice' subsection under Preliminary Process Synthesis. The selectivity and conversion of propane and propylene were taken from US Patent 324,778[3]. This patent did not give a specific breakdown for the selectivity of benzene, toluene and xylene so a split of 35% benzene, 45% toluene, and 20% xylene was used.[19]

*Posttreatment*

The reactor effluent will move to Section 200 to separate the light components but its temperature must be reduced in order to prevent damage to the multistage compressors, C-201 and C-202. The stream entering the multistage compressors must be less than 110$^{o}$F. The reactor effluent, S-107, passes through the tube side of the shell and tube heat exchanger, H-101, where it is cooled to a safe temperature of 103$^{o}$F.

*Regeneration of Catalyst*

Coke builds up on the catalyst through its operation. This coke reduces the conversion of the reactant and the catalyst must be regenerated to maintain continuous and consistent production of BTX.

The procedure to regenerate the platinum-germanium zeolite catalyst has been provided in Patent US20080154079 A1.[6] There are five stages to the regeneration process. The first stage and second stage remove coke and sulfur from the catalyst via oxidation. The third stage redisperses platinum on the surface of the catalyst by using chlorine gas. The fourth stage removes chlorine and binds platinum to the surface of the zeolite by steaming. The fifth stage reduces the catalyst in hydrogen. Chlorine, water vapor, oxygen, hydrogen and the nitrogen are fed in different ratios to accomplish each step. The conditions of the reactor and the feed are shown in Table 17. Valves V-108, V-109, V-111, and V-113, control the quantity of reagent fed to the reactor that requires catalyst regeneration. Chlorine is stored on-site in pressure vessel, PV-101; water is vaporized in the column after being pumped by pump P-101; and all other gases are supplied by local pipelines.

Table 17. Time duration, temperature and mass flow rate of each reagent used in each stage of the regeneration process.

| **Stage** | **Time Duration (hr)** | **Temp ($^{o}$F)** | **Mass Flow (lb/hr)** | | | | |
|---|---|---|---|---|---|---|---|
| | | | **Chlorine** | **Water Vapor** | **Oxygen** | **Hydrogen** | **Nitrogen** |
| 1 | 24 | 1022 | 797 | 1613 | 3594 | 0 | 69300 |
| 2 | 24 | 1022 | 335 | 678 | 3594 | 0 | 27300 |
| 3 | 48 | 1022 | 3140 | 1610 | 8570 | 0 | 64000 |
| 4 | 12 | 1022 | 0 | 1610 | 8570 | 0 | 65300 |
| 5 | 24 | 1022 | 0 | 0 | 0 | 4710 | 9370 |

One regeneration cycle takes five and a half days to complete and so a Gantt chart was created to determine the minimum number of reactors necessary for continuous operation. The Gantt chart is shown in Figure 11. From this chart, it was determined that three reactors would be necessary for continuous operation.

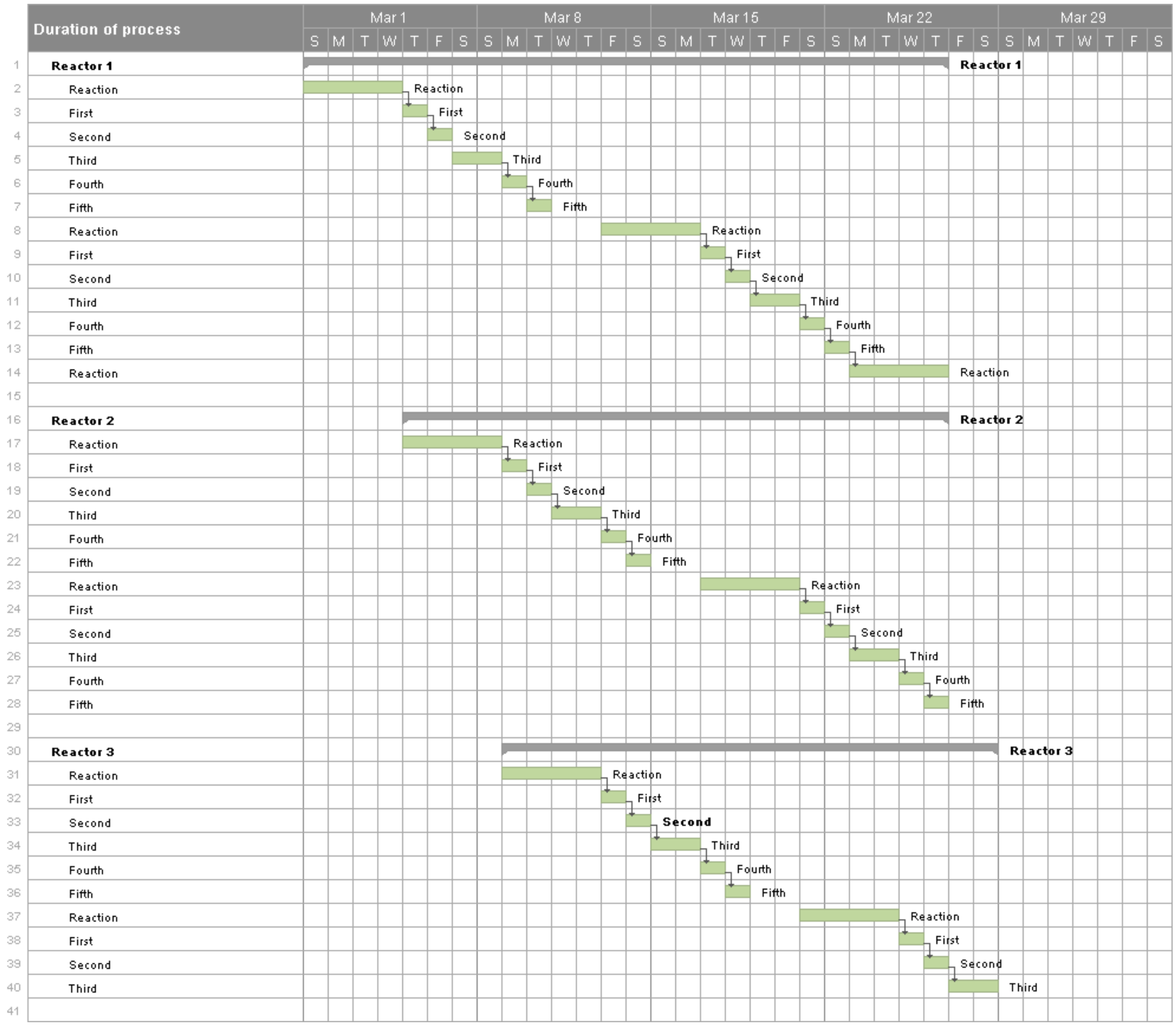


Figure 11. Gantt chart for the regeneration process. 'Reaction' represents the period in which the reactor is in operation. "First", "Second", "Third", "Fourth", and "Fifth" represent the different stages of the regeneration process.[20]

## Section 2 - Separation of Hydrogen and Light Hydrocarbons

This section separates the reaction products from Section 1 in stream S-108 into stream S-219, comprised of hydrogen and methane, that will be used to satisfy heating requirements around the plant; stream S-218, which is mainly C2 and C3 hydrocarbons that will be recycled to the reactor; and stream S-

210, which has a mix of all components except hydrogen and methane that will require further separation in Section 3.

*Compression*

In order to utilize the PRISM Separation system, PR-201, the feed must be at a pressure of 700 psia. Stream S-108 first enters two parallel multistage compressors, C-201 and C-202. Each compressor is comprised of four stages. Each compression stage's output pressure is 2.47 times the input pressure. Between each stage, the contents are cooled to 104 $^{o}$F using cooling water. As a result, each stage becomes saturated and liquid is recovered as streams S-202, S-203 and S-204. The output stream, S-201, is also saturated and so must be fed to a flash vessel, COL-201, to separate the liquid phase from the vapor phase. The liquid streams leaving the multistage compressors and the liquid stream leaving the flash vessel (S-202, S-203, S-204 and S-205) will be fed to a distillation column that is operating at a pressure of 100 psia. Before mixing, all the streams must be at the same pressure. Stream S-204 is lower than the required pressure so it is fed through a pump, P-201. On the other hand, the other streams are higher than the required pressure so they are fed through valves to expand the stream to the desired pressure. The streams are then mixed to form Stream S-210 and sent to stage 3.

*Pretreatment*

Before feeding the light stream S-211, to the PRISM Unit PR-201, the temperature must be increased to 181$^{o}$F. This was accomplished through a network of heat exchangers. The vapor stream of COL-201, stream S-211, is fed into the shell side of the heat exchanger H-201. The hot stream entering H-201, Stream S-315, is the distillate of the distillation column, COL-302. The hot stream cools to 136$^{o}$F and is sent to the three one-day storage tanks, ST-201, ST-202 and ST-203. The cold stream, S-212, exits at 115$^{o}$F and goes into the next heat exchanger, H-202. This heat exchanger uses the bottoms product of the distillation column, COL-302, in the tube side at a temperature of 384$^{o}$F. The hot stream exits at 133$^{o}$F and is then fed to three one-day storage tanks, ST-204, ST-205, and ST-206. The vapor stream exits the shell side of H-202 at 120$^{o}$F to be fed into the final shell and tube heat exchanger, H-203. This heat exchanger heats the gas to 181$^{o}$F by using steam generated by the steam boilers, F-401 through F-407. The steam condenses and leaves in Stream S-217 where the water is recycled to the steam boiler. The light hydrocarbon stream, S-214, is now at a temperature of 181$^{o}$F and a pressure of 700 psia, which are suitable conditions for the PRISM system, PR-201.

*PRISM Unit*

The PRISM Unit is responsible for separating hydrogen from the vapor stream. It accomplishes this using membrane technology. At the conditions of Stream S-214, the permeate of the PRISM system, S-219, will recover 85% of the hydrogen in Stream S-214 and will have a purity of 72% hydrogen with the balance being methane. The hydrogen recovered is at a pressure of 200 psia. The permeate is split by the valve V-206 and the gas is sent to each furnace to provide the required heat to operate the unit.

## Section 3 - Separation of BTX Product and Heavier Hydrocarbons

The primary purpose of this section is to separate the liquid feed, S-210, into light components that will be recycled to the reactor; the BTX product; and heavier hydrocarbons that will be sold as a gasoline blend.

COL-301 is a 65 stage separation column that treats propane as the light key and benzene as the heavy key. First the stream S-210 enters COL-301 above stage 22. Each stage was assumed to have a Murphree tray efficiency of 65%. The vapor stream, S-301 exits the column at a temperature of 209$^{o}$F and a pressure of 93 psia. It then passes through a partial condenser COND-301 that uses cooling water to condense the stream. The saturated mixture then enters a reflux accumulator, RA-301. The mass reflux ratio is set to 0.103 and the mass distillate to feed ratio is set to 0.140. The distillate leaves the reflux accumulator as stream S-305 to be recycled to the reactors while the liquid is pumped by pump P-301 back into the column. Liquid leaves the bottom of the column at a temperature of 340$^{o}$F and a pressure of 102 psia as stream S-306. The liquid is pumped by pump P-302 and is fed to a kettle reboiler, RB-301. The boil-up ratio of the reboiler is 1.08 and the bottoms to feed ratio is 0.858. The contents of the partial reboiler are vaporized by steam obtained from S-408. The steam condenses and returns to the steam boilers, F-401 through F-407, in Stream S-308. The vapor stream S-309 is recycled back to the column and the liquid is taken from S-310.

The bottoms product of the first column then enters the second distillation column, COL-302. This column has 42 stages and it accepts the feed above tray 23. This distillation column was had a Murphree tray efficiency of 65%. Stream S-311, the vapor recovered from the top of the column, is at a temperature of 241$^{o}$F and a pressure of 26 psia. Stream S-311 passes through a total condenser where it is cooled to a temperature of 200$^{o}$F and the liquid is fed to a reflux accumulator, RA-302. The mass reflux ratio of the condenser is 0.642 and the distillate to feed ratio is set to 0.907. The distillate is recovered as S-315 and is sent to the heat exchanger S-202 and the reflux is pumped by pump P-303 and returned to the column. The liquid from the bottom of the column leaves as a temperature of 387$^{o}$F and a pressure of 32 psia. The liquid is pumped by P-304 to a reboiler, RB-302. Steam from the steam boilers, F-401 through F-407, satisfies the heat requirements of the reboiler. After it condenses, it returns to the steam boilers to be evaporated again. The reboiler operates at a mass boil up ratio of 15.9 and a bottoms to feed ratio of 0.093. The vapor returns to the column as stream S-318 and the gasoline-blend product goes to heat exchanger H-202 to be cooled.

## Section 4 - Steam Generation

This section of the process satisfies all the heating requirements of the plant aside from those of the reactor. Water at ambient conditions is pumped to the pressure of the recycled stream using pump P-401. Steam from heat exchanger H-203 and reboilers RB-301 and RB-302 is mixed with the liquid water and fed to seven steam boilers, F-401 through F-407. The furnaces are heated by combusting hydrogen and methane from the permeate of the PRISM unit, PR-201. The hydrogen and methane are combusted with 20% excess oxygen and the combustion products leave the boilers at a temperature of 572$^{o}$F. The heat generated produces high pressure steam, S-404. However, not all the steam is needed to satisfy the plant's utility requirements. Steam S-405 represents steam that is sold. The temperature of the steam is too high for the plant's needs and so it is passed through a turbine, T-401 to adjust the pressure and temperature to more suitable conditions of 398$^{o}$F and 240 psia. Some electrical energy is recovered in the process that is used to drive the compressors, C-201 and C-202.

# Energy Balance and Utility Requirements

The proposed utility requirements have been designed to use all recovered heat and electricity to reduce the total utility cost. Leftover requirements were fulfilled with either cooling water or steam.

## Steam Integration

Stream S-401 is cooling water pressurized with P-401/P-402 and mixed with leftover steam from heat exchanger H-203, and reboilers RB-301 and RB-302. The mixed stream, S-403, is in the liquid phase with a temperature of 106$^{o}$F and 230 psia. The fuel for the fired heaters is a mixture of S-221, containing methane and hydrogen, and S-410, containing oxygen and nitrogen for the combustion of S-221's gases. The heat produced from F-401 through F-407 is 1,280 MMBtu/hr and will be used to transfer heat to S-403 to produce steam. The outlet steam in S-404 is split at V-405 to sell approximately 1,015,660 lb/hr of the steam at 464$^{o}$F and 465 psia. The leftover steam, containing 452 MMBtu/hr, is sent through turbine T-401 to generate electricity and then split again to fulfill utility requirements to RB-301, RB-302, and H-203.

## Reactor Duty

The heat recovery section of the reactor, represented by heat exchanger H-101 and fired heater F-101, meets the utility requirements of reactors R-101, R-102, and R-103. H-101 will transfer 461 MMBtu/hr of heat to inlet stream S-105, allowing it to reach a temperature of 1148$^{o}$F. F-101 will allow S-106 to reach the operating temperature of 1350$^{o}$F and keep the reactors at an isothermal temperature of 1350$^{o}$F. The heat duty required by F-101 is 205.9 MMBtu/hr.

## Cooling Water

The process uses cooling water as the only external cooling source. Cooling water is used in condensers COND-301 and COND-302 to condense the vapors from the top of the columns. It is also used in the multistage condensers to cool the pressurized gas to 104$^{o}$F so that the heavier components may be separated as a liquid. Table 18 summarizes the amount of energy removed from the hot stream by the cooling water.

Table 18. Energy requirements for condensers and compressors.

| Equipment | Source | Energy Requirement (Btu/hr) |
|---|---|---|
| COND-301 | Cooling Water | 548155 |
| COND-302 | Cooling Water | 33077700 |
| C-201, C-202 (Combined) | Cooling Water | 181261000 |

## Electricity

This process uses several pieces of equipment that consume and generate electricity. Pumps and compressors are required throughout the plant to account for the pressure drop along pipes and through equipment. To mitigate the electricity costs for these units, turbines are installed when a vapor could be expanded. Table 19 shows a summary of the electricity required and supplied by each unit.

Table 19. Electricity requirement for pumps, turbines, and compressors. Note that a negative electricity requirement indicates that electricity is being generated.

| Equipment | Number of Units | Electricity Requirement per unit (hp) | Total Electricity Requirement (hp) |
|---|---|---|---|
| C-201<br>C-202 | 2 | 29985 | 59970 |
| P-101 | 1 | 0.0237 | 0.0237 |
| P-201 | 1 | 4.86 | 4.86 |
| P-202 | 1 | 2.08 | 2.08 |
| P-301 | 1 | 0.0393 | 0.0393 |
| P-302 | 1 | 4.85 | 4.85 |
| P-303 | 1 | 6.03 | 6.03 |
| P-304 | 1 | 4.04 | 4.04 |
| P-401 | 1 | 321 | 321 |
| T-101<br>T-102<br>T-103 | 3 | -4090 | -12270 |
| T-104 | 1 | -2564 | -2564 |
| T-105 | 1 | -93.5 | -93.5 |
| T-401 | 1 | -1470 | -1470 |
| **Net Requirement** | | | 43915 |

## Heat Exchanger Network

This process consumes a tremendous amount of energy. A heat exchanger network was drawn to determine streams that could transfer energy in order to economically minimize external heating and cooling utilities. Figure 12 shows the process' heat exchanger network. Tables 19 through 30 show the design specifications of the heat exchangers and temperatures of the streams interacting with the entering and leaving the heat exchangers. Appropriate overall heat transfer coefficients, U, were obtained from Product and Process Design Principles[14].

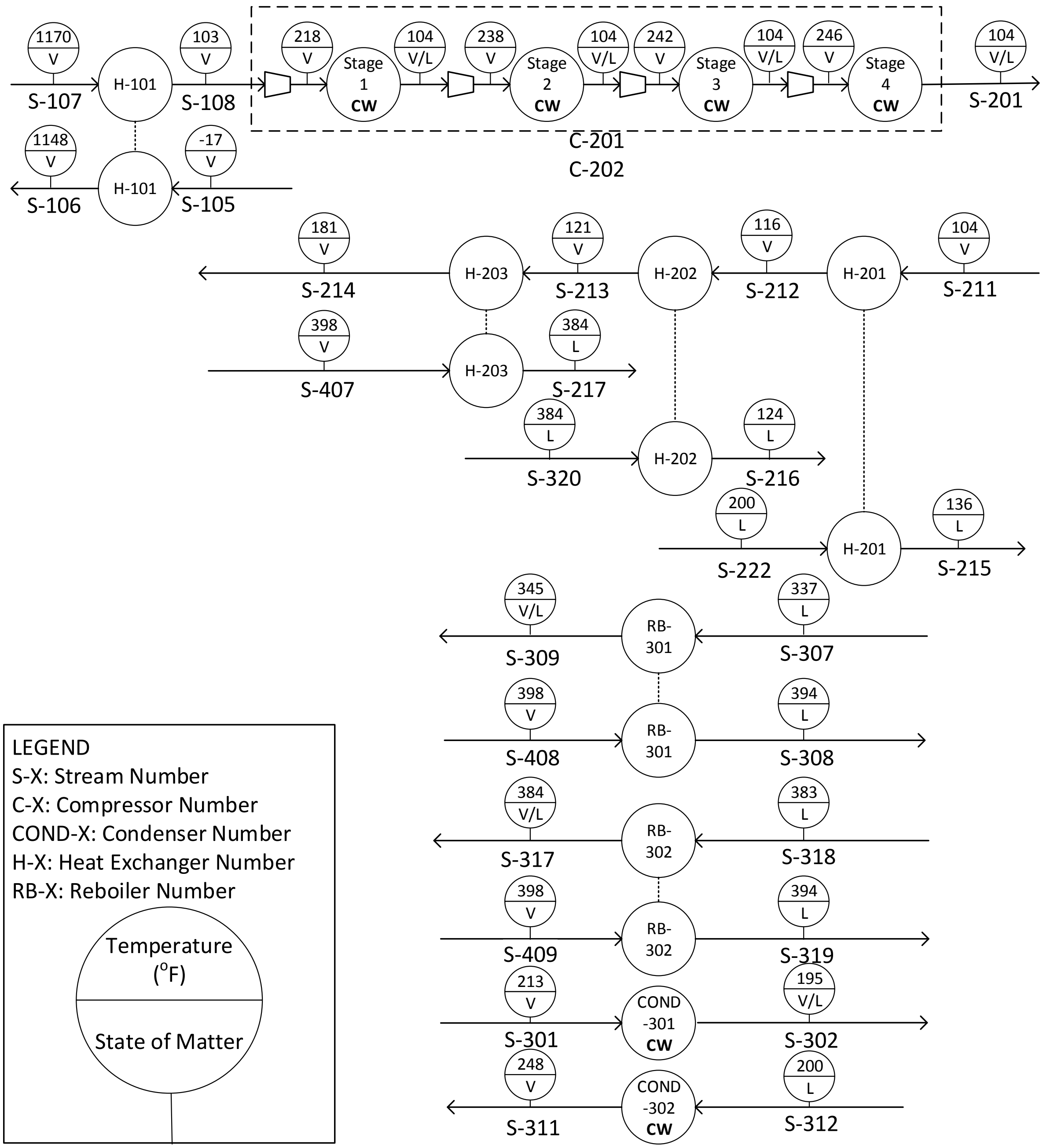


Figure 12. Heat Exchanger Network for the Process.

Tables 19-30. Heat Exchanger Network Tables.

| Unit | H-101 | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^oF$)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-107 | 1170 | 149.7 | 461.3 |
| Hot out | S-108 | 103 | | |
| Cold in | S-105 | -17 | **Area (ft$^2$)** | **LMTD ($^oF$)** |
| Cold out | S-106 | 1148 | 53340 | 57.8 |

| Unit | C-101 Stage 1 | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^oF$)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-108 | 218 | 149.7 | 446.3 |
| Hot out | S-108 | 104 | | |
| Cold in | CW | 90 | **Area (ft$^2$)** | **LMTD ($^oF$)** |
| Cold out | CW | 120 | 7166 | 43.2 |

| Unit | C-101 Stage 2 | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^oF$)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-108 | 238 | 149.7 | 46.32 |
| Hot out | S-108 | 104 | | |
| Cold in | CW | 90 | **Area (ft$^2$)** | **LMTD ($^oF$)** |
| Cold out | CW | 120 | 6342 | 48.8 |

| Unit | C-101 Stage 3 | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^oF$)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-108 | 242 | 149.7 | 44.78 |
| Hot out | S-108 | 104 | | |
| Cold in | CW | 90 | **Area (ft$^2$)** | **LMTD ($^oF$)** |
| Cold out | CW | 120 | 5996 | 49.9 |

| **Unit** | **C-101 Stage 4** | | | |
|---|---|---|---|---|
| | Stream | Temperature (°F) | **U (Btu/hr-ft²-°F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-108 | 246 | 149.7 | 44.07 |
| Hot out | S-108 | 140 | | |
| Cold in | CW | 90 | **Area (ft²)** | **LMTD (°F)** |
| Cold out | CW | 120 | 3580 | 82.2 |

| **Unit** | **H-201** | | | |
|---|---|---|---|---|
| | Stream | Temperature (°F) | **U (Btu/hr-ft²-°F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-222 | 196 | 149.7 | 3.492 |
| Hot out | S-215 | 136 | | |
| Cold in | S-211 | 104 | **Area (ft²)** | **LMTD (°F)** |
| Cold out | S-212 | 115 | 433.6 | 53.9 |

| **Unit** | **H-202** | | | |
|---|---|---|---|---|
| | Stream | Temperature (°F) | **U (Btu/hr-ft²-°F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-320 | 384 | 149.7 | 1.453 |
| Hot out | S-216 | 133 | | |
| Cold in | S-212 | 115 | **Area (ft²)** | **LMTD (°F)** |
| Cold out | S-213 | 120 | 133.0 | 73.0 |

| **Unit** | **H-203** | | | |
|---|---|---|---|---|
| | Stream | Temperature (°F) | **U (Btu/hr-ft²-°F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-407 | 398 | 149.7 | 17.14 |
| Hot out | S-217 | 384 | | |
| Cold in | S-213 | 120 | **Area (ft²)** | **LMTD (°F)** |
| Cold out | S-214 | 181 | 478.5 | 239 |

| **Unit** | **RB-301** | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^o$F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-408 | 398 | 149.7 | 19.51 |
| Hot out | S-308 | 394 | | |
| Cold in | S-307 | 340 | **Area (ft$^2$)** | **LMTD ($^o$F)** |
| Cold out | S-309 | 349 | 2371 | 55.0 |

| **Unit** | **RB-302** | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^o$F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-409 | 398 | 149.7 | 24.69 |
| Hot out | S-319 | 394 | | |
| Cold in | S-317 | 387 | **Area (ft$^2$)** | **LMTD ($^o$F)** |
| Cold out | S-318 | 387 | 13260 | 12.4 |

| **Unit** | **COND-301** | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^o$F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-301 | 209 | 149.7 | 0.507 |
| Hot out | S-302 | 186 | | |
| Cold in | CW | 90 | **Area (ft$^2$)** | **LMTD ($^o$F)** |
| Cold out | CW | 120 | 150 | 98.9 |

| **Unit** | **COND-302** | | | |
|---|---|---|---|---|
| | Stream | Temperature ($^oF$) | **U (Btu/hr-ft$^2$-$^o$F)** | **Heat duty (MMBTU/hr)** |
| Hot in | S-311 | 241 | 149.7 | 33.19 |
| Hot out | S-312 | 196 | | |
| Cold in | CW | 90 | **Area (ft$^2$)** | **LMTD ($^o$F)** |
| Cold out | CW | 120 | 1867 | 119 |

# Equipment List and Unit Descriptions

## Compressors

C-201 and C-202 are two cast iron/carbon-steel centrifugal compressors in parallel. These compressors raise the pressure of stream S-108, the cooled product stream leaving the reactor, from 26 psia to 730 psia. The compressors will run at an isentropic efficiency of 80% and will each require 29,990.65 hp of electricity. The exit streams from the compressor will experience a small temperature drop from 106$^o$F to 104$^o$F. The bare module costs for C-201 and C-202 are each $18,221,846.

## Condensers

COND-301 is a condenser for column COL-301. COND-301 is designed as a shell-and-tube, floating-head heat exchanger composed of carbon steel. The tube-side fluid is stream S-301, the vapor stream exiting the top of COL-301, and it is cooled from 209$^o$F to 186$^o$F at an outlet pressure of 83 psia. The shell-side fluid is cooling water that is supplied externally from the process. The tube length is 20 ft and has a surface area of 150 ft$^2$. The shell-side pressure is kept at 83 psig. COND-301 has an overall heat transfer coefficient of 250 Btu/hr-ft$^2$-$^o$F and has a heat duty of 0.548 MMBtu/hr. The bare-module cost of COND-301 is $57,297.

COND-302 is a condenser for column COL-302. COND-302 is designed as a shell-and-tube, floating-head heat exchanger composed of carbon steel. The tube-side fluid is stream S-311, the vapor stream exiting COL-302, and it is cooled from 241$^o$ F to 196$^o$ F at an outlet pressure of 16 psia. The shell-side fluid is cooling water that is supplied externally from the process. The tube length is 20 ft and has a surface area of 4265 ft$^2$. The shell-side pressure is kept at 2.3 psig. COND-302 has an overall heat transfer coefficient of 250 Btu/hr-ft$^2$-$^o$F and has a heat duty of 33.1 MMBtu/hr. The bare-module cost of COND-302 is $174,664.

## Distillation Columns and Flash Vessels

COL-201 is a single sieve tray, carbon steel flash vessel that separates S-201 into vapor and liquid streams. S-201 is the stream exiting the multistage compressor. The vapor product will be sent to the PRISM separation unit, PR-201, to separate hydrogen and methane from the C2 and C3 hydrocarbons. The liquid product proceeds to Section 3 of the process for further separation. The column has a height of 15.5 ft, a diameter of 4.92 ft, a wall thickness of 1.93 inch, and a weight of 24,464 lb. It operates at 715.3 psig. The bare module cost of COL-301 is $496,260.

COL-301 is a sieve tray, carbon steel distillation tower into which stream S-210 is fed. S-210 consists of the heavier streams that left the multistage compressors (C-201 and C-202) between each compression stage as well as the liquid stream that left the flash vessel (COL-201). The bottoms product of COL-301 consists primarily of C6+ hydrocarbons that are sent to COL-302 for further separation. The distillate consists of lighter hydrocarbons that are recycled back to the reactor. There are 65 carbon steel trays, with the feed location at tray 22. The column is operated at a mass reflux ratio of 0.103. The column has a height of 112 ft, a diameter of 2.28 ft, a wall thickness of 1.13 in, and a weight of 38,899 lb. It operates at 87.8 psig. The bare module cost of COL-301 is $946,960.

COL-302 is a sieve tray, carbon steel distillation tower into which the bottoms product of COL-301 is fed in order to separate the C9+ hydrocarbons from the BTX product. The distillate product and the bottoms product are fed through heat exchangers H-201 and H-202 respectively to reduce their temperature to appropriate levels for storage. COL-302 contains 42 carbon steel trays, with the feed location at tray 25. The column is operated at a mass reflux ratio of 0.642. The column has a height of 77 ft, a diameter of 9.14 ft, a wall thickness of 0.563 in, and a weight of 55,923 lb. It operates at 18 psig. The bare module cost of COL-302 is $1,422,607.

## Fired Heaters

F-101 represents the section of the heat recovery unit that will raise the temperature of the feed to the reactor to the appropriate reaction conditions after heat exchange with the reactor outlet occurs. The bare module cost and utility requirements of the entire heat recovery section are included in the cost and requirements for the reactor units R-101, R-102, and R-103.

F-401 through F-407 are steam boilers that will take S-403 and produce steam to fulfill heating requirements for multiple units in the process. S-403 comes from V-403 and will have a pressure increase of 230 psia to 465 psia and a temperature change of 106$^{o}$F to 1350$^{o}$F. The fired heater has a heat duty of 1,280 MMBtu/hr. The bare module cost of each unit is $1,526,030.

## Heat Exchangers

H-101 represents the section of the heat recovery unit that will exchange heat between the feed and the effluent streams of the reactor unit. The bare module cost and utility requirements of the entire heat recovery section are included in the cost and requirements for the reactor units R-101, R-102, and R-103.

H-201 is a floating-head shell-and- tube heat exchanger that will partially pre-heat stream S-211 to prepare for the PRISM separation unit, PR-201. S-211 is the vapor stream leaving the flash vessel (COL-201). This stream is on the shell side and will be heated from 104$^{o}$F to 116$^{o}$F with a pressure drop of 10 psia. The tube-side fluid is the distillate from COL-301, S-315, which is cooled from 200$^{o}$F to 136$^{o}$F with a pressure drop of 10 psia. The heat exchanger is composed of carbon steel for both the tube and shell side. The tube length of H-201 is 20 ft with a surface area of 430.9 $ft^2$. The shell-side pressure will be kept at 705.3 psig. H-201 has an overall heat transfer coefficient of 149.7 Btu/hr-$ft^2$-$^oF$ and will transfer 3.28 MMBtu/hr of heat. The bare-module cost of the heat exchanger is $78,762. No external utilities will be required for H-201.

H-202 is a floating-head shell-and-tube heat exchanger that will continue to pre-heat S-211 to reach the PRISM unit's operating temperature. The shell-side fluid is the outlet stream, S-212, from heat exchanger H-201 that is heated from 116$^o$ F to 121$^o$ F with a pressure drop of 10 psia. The tube-side fluid is S-320, the bottoms product of COL-302, which is cooled from 384$^o$F to 124$^o$F. The heat exchanger is composed of carbon steel for both the tube and shell side. The tube length of H-202 is 20 ft with a surface area of 150 $ft^2$. The shell-side pressure will be kept at 695.3 psig. H-202 has an overall heat transfer coefficient of 149.7 Btu/hr-$ft^2$-$^oF$ and will transfer 1.49 MMBtu/hr of heat. The bare-module cost of the heat exchanger is $68,821. No external utilities will be required for H-202.

H-203 is a shell-and-tube heat exchanger that will raise S-213's temperature to the temperature of the PRISM unit. The shell-side fluid is the outlet shell-side stream from H-202, S-213, and is heated from 121$^o$F to 181$^o$F with a pressure drop of 10 psia. The tube-side fluid is S-407, which is a fraction of the steam from boilers F-401 through F-407. It is condensed with a temperature drop of 398$^o$ F to 384$^o$ F and has a pressure drop of 10 psia. The heat exchanger is composed of carbon steel for both the tube and shell side. The tube length of H-203 is 20 ft and has a surface area of 478.6 $ft^2$. The shell-side pressure will be kept at 685.3 psig. H-203 has an overall heat transfer coefficient of 149.7 Btu/hr-$ft^2$-$^oF$ and will transfer 17.3 MMBtu/hr of heat. The bare-module cost of the heat exchanger is $80,482. No external utilities will be required for H-203.

## Pressure Vessel

PV-101 is a spherical pressure vessel that stores the chlorine gas used in the regeneration process. The vessel is modeled as a carbon steel storage tank due to its low vapor pressure, as suggested by Dr. Richard Bockrath. The vessel stores sufficient chlorine for one regeneration cycle, or 480,839 gallons of chlorine. The bare module cost of PV-101 is $1,270,743.

## PRISM Unit

PR-201 is a commercial membrane separation system that will separate methane and hydrogen from the lighter hydrocarbons products in stream S-214. The operating temperature and pressure of PR-201 are 181$^o$F and 200 psia, respectively. At these conditions, the system will recover 85% of the hydrogen from the feed and will have a purity of 72% hydrogen, with the balance being methane. The cost of PR-201 is $17,000,000, as suggested by Karin Fair from Air Products and Chemicals, Inc.

## Pumps

P-201 is a cast-iron centrifugal pump that will raise the pressure of stream S-204, the first stream to leave the multistage compressors, from 55 psia to 100 psia. This pump is required as the streams coming from the compressors (C-201 and C-202) and the flash vessel (COL-201) must be at the same pressure when mixed to form the feed to COL-301. The pump has a volumetric flow rate of 148.5 gpm and generates a head of 125 ft. The electricity requirement for P-201 is 4.859 hp at an efficiency of 80%. The bare module cost of P-201 is $12,308. An additional pump with the same specifications and cost will be purchased as a backup for the primary pump.

P-301 is a cast iron centrifugal pump that will raise the pressure of stream S-303 from 83 psia to 93 psia. This pump is required for raising the stream coming from reflux accumulator RA-301 to COL-301's operating pressure. The pump has a volumetric flow rate of 5.39 gpm and generates a head of 29.6 ft. The electricity requirement for P-301 is 0.0392 hp at an efficiency of 80%. The bare module cost of P-301 is $11,053. An additional pump with the same specifications and cost will be purchased as a backup for the primary pump.

P-302 is a cast iron centrifugal pump that will raise the pressure of stream S-306, the bottoms product of COL-301, from 102 psia to 109 psia. This pump is required to raise S-306 to the reboiler RB-301's operating pressure. The pump has a volumetric flow rate of 749 gpm and generates a head of 21.9 ft. The electricity requirement for P-302 is 3.658 hp at an efficiency of 80%. The bare module cost of P-302 is $14,602. An additional pump with the same specifications and cost will be purchased as a backup for the primary pump.

P-303 is a cast iron centrifugal pump that will raise the pressure of stream S-313, the reflux stream returning to COL-302 from RA-302, from 16 psia to 26 psia. This pump is required to raise S-313 to column COL-302's operating pressure. The pump has a volumetric flow rate of 285 gpm and generates a head of 83.7 ft. The electricity requirement for P-303 is 6.03 hp at an efficiency of 80%. The bare module cost of P-303 is $11,692. An additional pump with the same specifications and cost will be purchased as a backup for the primary pump.

P-304 is a cast iron centrifugal pump that will raise the pressure of stream S-316, the bottoms product of COL-302, from 32 psia to 37 psia. This pump is responsible for raising S-316 to the reboiler RB-302's operating pressure. The pump has a volumetric flow rate of 555 gpm and generates a head of 32.9 ft. The electricity requirement for P-304 is 4.04 hp at an efficiency of 80%. The bare module cost of P-304 is $14,731. An additional pump with the same specifications and cost will be purchased as a backup for the primary pump.

P-401 is a cast iron centrifugal pump. These pumps will raise the pressure of stream S-401 from 14.5 psia to 230 psia. This pump is required to allow the streams S-217, S-308, S-317 to be at the same pressure when mixing occurs for fired heaters F-401 and F-402. The pump has a volumetric flow rate of 2040 gpm and generates a head of 500 ft. The electricity requirement for P-401 is 321 hp at an efficiency of 80%. The bare module cost of P-401 is $49,893. An additional pump with the same specifications and cost will be purchased as a backup for each primary pump.

## Reactors

R-101, R-102, and R-103 compose a group of three steam reforming reactors for the conversion of ethane to BTX, in which the feed is passed through tubes packed with catalyst. Direct fired heating is used on the outsides of the tubes to maintain a constant reaction temperature of 1170°F. The model will be purchased from Jacobs Engineering Group at a total installed cost of $55 million per unit, including a heat recovery section in which the outlet stream is heat exchanged with the inlet stream. The dimensions of a single reactor, including the heat recovery section and all civil and structural works, are a length of 95 ft, width of 59 ft, and a height of 105 ft. Three reactors are used to ensure that at least one reactor will be operating at all times, while the other two are either regenerating or on standby. Each reactor will operate in production mode for 5 days, regeneration mode for 5.5 days, and standby mode for 1.5 days. Standby time is required to ensure that only one reactor is producing BTX at a time, preventing fluctuation in flow rate at the outlet of the reactor section.

The highly endothermic reaction converts ethane to BTX as well as smaller hydrocarbons (e.g., methane, propane, propylene, and ethylene), trimethylbenzene, and hydrogen. The C2 and C3 hydrocarbons are recycled to produce a higher yield of BTX. The catalyst used is Pt/Ge/ZSM-5 (604,223 lb). The inlet to the reactor, S-106, has a mass flow rate of 570,023 lb/hr at 1166$^{o}$ F and 43.7 psia. The outlet from the reactor, S-107, has a mass flow rate of 570,023 lb/hr at 1166$^{o}$F and 36.4 psia. The adiabatic temperature drop across the reactor is 627°F and the heat duty is 103 MMBtu/hr.

## Reboilers

RB-301 is a partial reboiler for column COL-301. This heat exchanger is designed as a shell-and-tube kettle vaporizer composed of carbon steel for both sides. The tube-side fluid is stream S-408, which is a fraction of the steam from the steam boilers F-401 through F-407. It condenses with a temperature drop of 398$^{o}$F to 394$^{o}$ F and an outlet pressure of 230 psia. The shell-side fluid is stream S-307, the liquid leaving the bottom of COL-301, which will be partially vaporized at an outlet pressure of 99 psia. The outlet is split into S-309, which is sent back to COL-301, and S-310, which is sent to H-202. The tube length is 20 ft and has a surface area of 1420 ft$^2$. The shell-side pressure is kept at 84.3 psig. RB-301 has an overall heat transfer coefficient of 250 Btu/hr-ft$^2$-$^{o}$F and has a heat duty of 19.5 MMBtu/hr. The bare-module cost of RB-301 is $148,379. All utilities are provided internally by the system, so no external utilities are required for RB-301.

RB-302 is a partial reboiler for column COL-302. This heat exchanger is designed as a shell-and-tube kettle vaporizer composed of carbon steel for both sides. The tube side is stream S-409, which is a fraction of the steam from the steam boilers F-401 through F-407. It condenses with a temperature drop of 398$^o$F to 394$^o$ F and an outlet pressure of 230 psia. The shell-side fluid is stream S-317, the liquid leaving the bottom of COL-302, which will be partially vaporized at an outlet pressure of 31 psia. The outlet is split into S-318, which is sent back to COL-302, and S-320, which is sent to H-202. The tube length is 20 ft and has a surface area of 571.7 ft$^2$. The shell-side pressure is kept at 16.3 psig. RB-301 has an overall heat transfer coefficient of 250 Btu/hr-ft$^2$-$^o$F and has a heat duty of 1.78 MMBtu/hr. The bare-module cost of RB-302 is $107,486. All utilities are provided internally by the system, so no external utilities are required for RB-302.

## Reflux Accumulators

RA-301 is a reflux accumulator for column COL-301. This piece of equipment is a horizontal vessel composed of carbon steel with a diameter of 18.3 ft, a length of 36.6 ft, a wall thickness of 0.978 inch, and a weight of 118,143 lb. The operating conditions for RA-301 are 83 psi and 195$^o$ F. The bare module cost of RA-301 is $663,053.

RA-302 is a reflux accumulator for column COL-302. This piece of equipment is a horizontal vessel composed of carbon steel with a diameter of 7.41 ft, a length of 14.8 ft, a wall thickness of 0.500 inch, and a weight of 9,907 lb. The operating conditions for RA-302 are 17 psi and 250 $^o$ F. The bare module cost of RA-302 is $133,482.

## Storage Tanks

ST-201 through ST-203 are storage tanks for the BTX product. The BTX product will enter the storage at 136$^o$F and 17 psia. Stream S-215 is split between three tanks and the mixture contains 70,269 lb/hr of benzene, 34,673 lb/hr of toluene, and 9,099 lb/hr of xylene. The storage tank has a floating roof and is composed of carbon steel. Each tank will contain 590,366 gal of BTX product. The bare module cost of each storage tank is $472,692.

ST-204 through ST-206 are storage tanks for the heavy hydrocarbon products. Stream S-216 goes into each storage tank and will enter at 136$^o$F and 17 psia. Stream S-216 contains approximately 11,661 lb/hr of heavy hydrocarbons. The storage tank has a floating roof and is composed of carbon steel. Each tank will contain 40,429 gal of BTX product. The bare module cost of each storage tank is $82,619.

## Turbines

T-101, T-102, and T-103 are power-recovery turbines that take the outlet stream, S-218, from the PRISM separation unit and convert the pressure discharge to electricity, with an isentropic efficiency of 80%. The turbines cause a pressure drop of 690 psia to 54 psia and a temperature drop of 181$^{o}$ F to -27$^{o}$ F. Each turbine produces approximately 4089.8 hp. The bare module cost of each turbine is $506,252.

T-104 is a power-recovery turbine that takes the ethane feedstock stream, S-101, and converts the pressure discharge to electricity, with an isentropic efficiency of 80%. The turbine causes a pressure drop of 265 psia to 54 psia and a temperature drop of 80$^{o}$ F to -37$^{o}$ F. These operating conditions produce approximately 2563.9 hp. The bare module cost of T-104 is $346,820.

T-105 is a power-recovery turbine that takes the outlet stream, S-305, from RA-301, which is the distillate product of COL-301. This turbine converts the pressure discharge to electricity, with an isentropic efficiency of 80%. The turbine causes a pressure drop of 83 psia to 54 psia and a temperature drop of 186$^{o}$ F to 165$^{o}$ F. These operating conditions produce approximately 95.9 hp. The bare module cost of T-104 is $24,222.

T-401 is a power-recovery turbine that takes the outlet stream, S-406, from V-405, which is a portion of the steam boilers' product stream. This turbine converts the pressure discharge to electricity with an isentropic efficiency of 80%. The turbine causes a pressure drop of 465 psia to 240 psia and a temperature drop of 464$^{o}$ F to 398$^{o}$ F. These operating conditions produce approximately 1466 hp. The bare module cost of T-401 is $220,567.

# Specification Sheets

## Compressors

| COMPRESSOR | | | | | |
|---|---|---|---|---|---|
| Identification: C-201, C-202 (Run in parallel) | | | | | |
| Function: Compresses the reactor outlet to 730 psia and condenses heavier species. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Feed | Exit 1 | Exit 2 | Exit 3 | Exit 4 |
| **Materials Handled** | S-108 | S-201 | S-202 | S-203 | S-204 |
| Hydrogen | 18388 | 18388 | Trace | Trace | Trace |
| Methane | 162584 | 161167 | 783 | 391 | 243 |
| Ethane | 209537 | 205548 | 2131 | 1135 | 723 |
| Ethylene | 22090 | 21752 | 182 | 95.5 | 60.5 |
| Propane | 9027 | 8615 | 217 | 119 | 76.5 |
| Propylene | 2774 | 2695 | 40.9 | 22.2 | 15.7 |
| Benzene | 88283 | 20942 | 20551 | 23052 | 23738 |
| Toluene | 35905 | 1654 | 4717 | 10593 | 18941 |
| P-Xylene | 9178 | 35.4 | 300 | 1726 | 7117 |
| 1,3,5-Trimethylbenzene | 11739 | 2.56 | 61.2 | 967 | 10708 |
| **Total Flow (lb/hr)** | 569504 | 440798 | 28984 | 38100 | 61622 |
| **Design Data** | | | | | |
| Construction Material | | Cast Iron/Carbon-Steel | | | |
| Drive | | Electric Motor Drive | | | |
| Consumed Power (hp) | | 71442 | | | |
| **Purchase Cost (for all units)** | | **$32,137,296.88** | | | |
| **Costing Information Source** | | **Product and Process Design Principles**[14] | | | |

## Condensers

| CONDENSER | | |
|---|---|---|
| Identification: COND-301 | | |
| Function: Partially condenses the vapor from the top of COL-301 from 213°F to 195°F | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-301 | S-302 |
| Hydrogen | Trace | Trace |
| Methane | 2723 | 2723 |
| Ethane | 7089 | 7089 |
| Ethylene | 612 | 612 |
| Propane | 720 | 720 |
| Propylene | 144 | 144 |
| Benzene | 10037 | 10037 |
| Toluene | 1186 | 1186 |
| P-Xylene | 42.8 | 42.8 |
| 1,3,5-Trimethylbenzene | Trace | Trace |
| **Total Flow (lb/hr)** | 22553 | 22553 |
| **Design Data** | | |
| Shell/Tube Material | Carbon Steel | |
| Tube Length (ft) | 20 | |
| Surface Area ($ft^2$) | 150 | |
| **Purchase Cost** | **$57,297.17** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| CONDENSER | | |
|---|---|---|
| Identification: COND-302 | | |
| Function: Condenses the vapor from the top of COL-302 from 248°F to 200°F | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-311 | S-312 |
| Benzene | 115357 | 115357 |
| Toluene | 56920 | 56920 |
| P-Xylene | 14998 | 14998 |
| 1,3,5-Trimethylbenzene | 66.5 | 66.5 |
| **Total Flow (lb/hr)** | 187342 | 187342 |
| **Design Data** | | |
| Shell/Tube Material | Carbon Steel | |
| Tube Length (ft) | 20 | |
| Surface Area ($ft^2$) | 4265 | |
| **Purchase Cost** | **$174,664.49** | |
| **Costing Information Source** | **Product and Process Design Principles** [14] | |

## Distillation Columns and Flash Vessel

| FLASH VESSEL | | | |
|---|---|---|---|
| Identification: COL-201 | | | |
| Function: Separates the saturated stream from the multistage compressors (C-201, C-202) into vapor and liquid streams. | | | |
| Operation: Continuous | | | |
| | **Mass Flow (lb/hr)** | | |
| | Feed | Exit 1 | Exit 2 |
| **Materials Handled:** | S-201 | S-211 | S-205 |
| Hydrogen | 18388 | 18388 | Trace |
| Methane | 161167 | 159866 | 1301 |
| Ethane | 205548 | 202499 | 3049 |
| Ethylene | 21752 | 21482 | 270 |
| Propane | 8615 | 8316 | 298 |
| Propylene | 2695 | 2630 | 64.2 |
| Benzene | 20942 | 9641 | 11301 |
| Toluene | 1654 | 397 | 1257 |
| P-Xylene | 35.4 | 3.73 | 31.6 |
| 1,3,5-Trimethylbenzene | 2.56 | Trace | 2.45 |
| **Total Flow (lb/hr)** | 440798 | 423224 | 17574 |
| **Design Data** | | | |
| Height (ft) | 15.5 | | |
| Inner Diameter (ft) | 4.92 | | |
| Wall Thickness (inches) | 1.93 | | |
| Design Pressure (psig) | 715.3 | | |
| Vessel Material | Carbon Steel | | |
| Tray/Packing | Tray | | |
| Tray Type | Sieve | | |
| Tray Material | Carbon Steel | | |
| Number of Trays | 1 | | |
| **Purchase Cost** | **$496,260.10** | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | |

| DISTILLATION COLUMN | | | | | |
|---|---|---|---|---|---|
| Identification: COL-301 | | | | | |
| Function: Takes the liquid streams from compressors (C-201, C-202) and separates C1-C3 from BTX compounds. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Feed 1 | Feed 2 (Reflux) | Feed 3 (Boil up) | Exit 1 | Exit 2 |
| **Materials Handled:** | S-210 | S-304 | S-309 | S-301 | S-306 |
| Hydrogen | Trace | Trace | Trace | Trace | Trace |
| Methane | 2717 | 5.39 | Trace | 2723 | Trace |
| Ethane | 7038 | 50.7 | Trace | 7089 | Trace |
| Ethylene | 608 | 3.61 | Trace | 612 | Trace |
| Propane | 711 | 9.08 | Trace | 720 | Trace |
| Propylene | 143 | 1.07 | Trace | 144 | Trace |
| Benzene | 78642 | 1664 | 104030 | 10037 | 174298 |
| Toluene | 35508 | 351 | 26936 | 1186 | 61609 |
| P-Xylene | 9175 | 19.1 | 4094 | 42.8 | 13244 |
| 1,3,5-Trimethylbenzene | 11739 | Trace | 3154 | Trace | 14893 |
| **Total Flow (lb/hr)** | 146280 | 2104 | 138214 | 22553 | 264044 |
| **Design Data** | | | | | |
| Height (ft) | 112 | | | | |
| Inner Diameter (ft) | 2.28 | | | | |
| Wall Thickness (inches) | 1.13 | | | | |
| Design Pressure (psig) | 114 | | | | |
| Vessel Material | Carbon Steel | | | | |
| Tray/Packing | Tray | | | | |
| Tray Type | Sieve | | | | |
| Tray Material | Carbon Steel | | | | |
| Number of Trays | 65 | | | | |
| Mass Reflux Ratio | 0.103 | | | | |
| Mass Distillate to Feed Ratio | 0.142 | | | | |
| **Purchase Cost** | **$835,061.31** | | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | | |

| DISTILLATION COLUMN | | | | | |
|---|---|---|---|---|---|
| Identification: COL-302 | | | | | |
| Function: Takes the bottoms product of COL-301 and separates BTX compounds from heavier hydrocarbons. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Feed | Feed (Reflux) | Feed (Boil up) | Exit 1 (Distillate) | Exit 2 (Bottoms) |
| **Materials Handled:** | S-310 | S-314 | S-318 | S-311 | S-316 |
| Benzene | 70269 | 70269 | Trace | 115357 | Trace |
| Toluene | 34673 | 34673 | Trace | 56920 | Trace |
| P-Xylene | 9151 | 9136 | 389 | 14998 | 404 |
| 1,3,5-Trimethylbenzene | 11739 | 40.5 | 182351 | 66.5 | 194050 |
| **Total Flow (lb/hr)** | 125831 | 114118 | 182741 | 187342 | 194453 |
| **Design Data** | | | | | |
| Height (ft) | 77 | | | | |
| Inner Diameter (ft) | 9.14 | | | | |
| Wall Thickness (inches) | 0.56 | | | | |
| Design Pressure (psig) | 26 | | | | |
| Vessel Material | Carbon Steel | | | | |
| Tray/Packing | Tray | | | | |
| Tray Type | Sieve | | | | |
| Tray Material | Carbon Steel | | | | |
| Number of Trays | 42 | | | | |
| Mass Reflux Ratio | 0.642 | | | | |
| Mass Distillate to Feed Ratio | 0.907 | | | | |
| **Purchase Cost** | **$1,422,606.78** | | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | | |

## Fired Heaters

| FIRED HEATER | | | | | |
|---|---|---|---|---|---|
| Identification: F-401, F-402, F-403, F-404, F-405, F-406, F-407 | | | | | |
| Function: Burns hydrogen and methane from the PRISM Unit to boil water to form high pressure steam for heating requirements. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Combustion Side | | | Water Side | |
| | Feed 1 | Feed 2 | Exit 1 | Feed 3 | Exit 2 |
| **Materials Handled:** | S-221 | S-410 | S-411 | S-403 | S-404 |
| Hydrogen | 18388 | 0 | 0 | 0 | 0 |
| Methane | 159866 | 0 | 0 | 0 | 0 |
| Water | 0 | 0 | 198009 | 1096360 | 1096360 |
| Oxygen | 0 | 299340 | 49890 | 0 | 0 |
| Nitrogen | 0 | 985838 | 985838 | 0 | 0 |
| Carbon Dioxide | 0 | 0 | 101223 | 0 | 0 |
| **Total Flow (lb/hr)** | 423224 | 1285180 | 1334960 | 1096360 | 1096360 |
| **Design Data** | | | | | |
| Subtype | Steam Boiler | | | | |
| Heat Duty (BTU/hr) | 191217482 | | | | |
| **Purchase Cost (for all units)** | **$10,682,210** | | | | |
| **Costing Information Source** | **Dr. Bockrath** | | | | |

## Heat Exchangers

| HEAT EXCHANGER | | | | |
|---|---|---|---|---|
| Identification: H-101 | | | | |
| Function: Exchange heat between the feed stream and the reactor outlet. | | | | |
| Operation: Continuous | | | | |
| | **Mass Flow (lb/hr)** | | | |
| | Feed 1 (Hot) | Exit 1 (Hot) | Feed 2 (Cold) | Exit 2 (Cold) |
| **Materials Handled:** | S-107 | S-108 | S-105 | S-106 |
| Hydrogen | 18388 | 18388 | 2758 | 2758 |
| Methane | 162584 | 162584 | 118810 | 118810 |
| Ethane | 209537 | 209537 | 389331 | 389331 |
| Ethylene | 22090 | 22090 | 22090 | 22090 |
| Propane | 9027 | 9027 | 14463 | 14463 |
| Propylene | 2774 | 2774 | 2774 | 2774 |
| Benzene | 88283 | 88283 | 18014 | 18014 |
| Toluene | 35905 | 35905 | 1232 | 1232 |
| P-Xylene | 9178 | 9178 | 27.5 | 27.5 |
| 1,3,5-Trimethylbenzene | 11739 | 11739 | Trace | Trace |
| **Total Flow (lb/hr)** | 569504 | 569504 | 569500 | 569500 |
| **Purchase Cost** | Included in R-101's cost. | | | |
| **Costing Information Source** | **Jacobs UK** | | | |

| HEAT EXCHANGER | | | | |
|---|---|---|---|---|
| Identification: H-201 | | | | |
| Function: Exchange heat between COL-201's vapor product and COL 302's vapor product. | | | | |
| Operation: Continuous | | | | |
| | **Mass Flow (lb/hr)** | | | |
| | Feed 1 (Hot) | Exit 1 (Hot) | Feed 2 (Cold) | Exit 2 (Cold) |
| **Materials Handled:** | S-315 | S-215 | S-211 | S-212 |
| Hydrogen | 0 | 0 | 18388 | 18388 |
| Methane | 0 | 0 | 159866 | 159866 |
| Ethane | 0 | 0 | 202499 | 202499 |
| Ethylene | 0 | 0 | 21482 | 21482 |
| Propane | 0 | 0 | 8316 | 8316 |
| Propylene | 0 | 0 | 2630 | 2630 |
| Benzene | 70269 | 70269 | 9641 | 9641 |
| Toluene | 34673 | 34673 | 397 | 397 |
| P-Xylene | 9136 | 9136 | 3.73 | 3.73 |
| 1,3,5-Trimethylbenzene | 40.5 | 40.5 | Trace | Trace |
| **Total Flow (lb/hr)** | 114118 | 114118 | 423224 | 423224 |
| **Design Data** | | | | |
| Subtype | Floating Head, Shell and Tube | | | |
| Shell/Tube Material | Carbon Steel/Carbon Steel | | | |
| Tube Length | 20 ft | | | |
| Surface Area ($ft^2$) | 430.917 | | | |
| Shell-Side Pressure (psig) | 705.3 | | | |
| **Purchase Cost** | $78,762.43 | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | |

| HEAT EXCHANGER | | | | |
|---|---|---|---|---|
| Identification: H-202 | | | | |
| Function: Exchange heat between H-201's shell side stream and COL 302's liquid product. | | | | |
| Operation: Continuous | | | | |
| | **Mass Flow (lb/hr)** | | | |
| | Feed 1 (Hot) | Exit 1 (Hot) | Feed 2 (Cold) | Exit 2 (Cold) |
| **Materials Handled:** | S-320 | S-216 | S-212 | S-213 |
| Hydrogen | 0 | 0 | 18388 | 18388 |
| Methane | 0 | 0 | 159866 | 159866 |
| Ethane | 0 | 0 | 202499 | 202499 |
| Ethylene | 0 | 0 | 21482 | 21482 |
| Propane | 0 | 0 | 8316 | 8316 |
| Propylene | 0 | 0 | 2630 | 2630 |
| Benzene | Trace | Trace | 9641 | 9641 |
| Toluene | Trace | Trace | 397 | 397 |
| P-Xylene | 14.7 | 14.7 | 3.73 | 3.73 |
| 1,3,5-Trimethylbenzene | 11698 | 11698 | Trace | Trace |
| **Total Flow (lb/hr)** | 11713 | 11713 | 423224 | 423224 |
| **Design Data** | | | | |
| Subtype | Floating Head, Shell and Tube | | | |
| Shell/Tube Material | Carbon Steel/Carbon Steel | | | |
| Tube Length | 20 ft | | | |
| Surface Area ($ft^2$) | 150 | | | |
| Shell-Side Pressure (psig) | 695.3 | | | |
| **Purchase Cost** | $68,821.01 | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | |

| HEAT EXCHANGER | | | | |
|---|---|---|---|---|
| Identification: H-203 | | | | |
| Function: Exchange heat between steam produced from F-401 through F-407 and H-202's shell side stream. | | | | |
| Operation: Continuous | | | | |
| | **Mass Flow (lb/hr)** | | | |
| | Feed 1 (Hot) | Exit 1 (Hot) | Feed 2 (Cold) | Exit 2 (Cold) |
| **Materials Handled:** | S-407 | S-217 | S-213 | S-214 |
| Hydrogen | 0 | 0 | 18388 | 18388 |
| Methane | 0 | 0 | 159866 | 159866 |
| Ethane | 0 | 0 | 202499 | 202499 |
| Ethylene | 0 | 0 | 21482 | 21482 |
| Propane | 0 | 0 | 8316 | 8316 |
| Propylene | 0 | 0 | 2630 | 2630 |
| Benzene | 0 | 0 | 9641 | 9641 |
| Toluene | 0 | 0 | 397 | 397 |
| P-Xylene | 0 | 0 | 3.73 | 3.73 |
| 1,3,5-Trimethylbenzene | 0 | 0 | Trace | Trace |
| Water | 22826 | 22826 | 0 | 0 |
| **Total Flow (lb/hr)** | 22826 | 22826 | 423224 | 423224 |
| **Design Data** | | | | |
| Subtype | Floating Head, Shell and Tube | | | |
| Shell/Tube Material | Carbon Steel/Carbon Steel | | | |
| Tube Length | 20 ft | | | |
| Surface Area ($ft^2$) | 478.5673 | | | |
| Shell-Side Pressure (psig) | 685.3 | | | |
| **Purchase Cost** | $80,482.61 | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | |

## Pressure Vessel

| PRESSURE VESSEL | |
|---|---|
| Identification: PV-101 | |
| Function: Stores a regeneration cycle's worth of chlorine. | |
| Operation: Batch | |
| | **Mass Flow (lb/hr)** |
| | Exit |
| **Materials Handled:** | S-113 |
| Chlorine | Varies based on regeneration stage. |
| **Total Flow lb/hr** | Varies based on regeneration stage. |
| **Design Data** | |
| Storage Capacity (gal) | 480839 |
| **Purchase Cost** | **$1,270,734.45** |
| **Costing Information Source** | **Product and Process Design Principles**[14] |

## PRISM Unit

| PRISM | | | |
|---|---|---|---|
| Identification: PR-201 | | | |
| Function: Separates hydrogen and methane from its feed stream, S-214, using membrane separation. | | | |
| Operation: Continuous | | | |
| | **Mass Flow (lb/hr)** | | |
| | Feed | Exit 1 | Exit 2 |
| **Materials Handled:** | S-214 | S-218 | S-219 |
| Hydrogen | 18388 | 2758 | 15630 |
| Methane | 159866 | 115104 | 44762 |
| Ethane | 202499 | 202499 | 0 |
| Ethylene | 21482 | 21482 | 0 |
| Propane | 8316 | 8316 | 0 |
| Propylene | 2630 | 2630 | 0 |
| Benzene | 9641 | 9641 | 0 |
| Toluene | 397 | 397 | 0 |
| P-Xylene | 3.73 | 3.73 | 0 |
| 1,3,5-Trimethylbenzene | Trace | Trace | 0 |
| **Total Flow (lb/hr)** | 423224 | 362832 | 60392 |
| **Purchase Cost** | **$17,000,000.00** | | |
| **Costing Information Source** | **Air Products and Chemicals, Inc.** | | |

## Pumps

| PUMP | | |
|---|---|---|
| Identification: P-101 | | |
| Function: Pumps water to R-101, R-102, or R-103, depending on which reactor is being regenerated. | | |
| Operation: Semi-continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-111 | S-112 |
| Water | Varies based on regeneration stage. | |
| **Total Flow lb/hr** | Varies based on regeneration stage. | |
| **Design Data** | | |
| Subtype | Centrifugal | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 3.24 | |
| Head (ft) | 23.2 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$15,500.06** | |
| **Costing Information Source** | **Product and Process Design Principles[14]** | |

| PUMP | | |
|---|---|---|
| Identification: P-202 | | |
| Function: Pumps the distillate product from COL-302 to H-201. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-315 | S-222 |
| Benzene | 70269 | 70269 |
| Toluene | 34673 | 34673 |
| P-Xylene | 9136 | 9136 |
| 1,3,5-Trimethylbenzene | 40.5 | 40.5 |
| **Total Flow (lb/hr)** | 114118 | 114118 |
| **Design Data** | | |
| Subtype | Centrifugal | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 289 | |
| Head (ft) | 28.9 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$10,818.20** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| PUMP | | |
|---|---|---|
| Identification: P-301 | | |
| Function: Pumps the liquid reflux from the reflux accumulator RA-301 to the distillation column, COL-301. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-303 | S-304 |
| Hydrogen | Trace | Trace |
| Methane | 5.39 | 5.39 |
| Ethane | 50.7 | 50.7 |
| Ethylene | 3.61 | 3.61 |
| Propane | 9.08 | 9.08 |
| Propylene | 1.07 | 1.07 |
| Benzene | 1664 | 1664 |
| Toluene | 351 | 351 |
| P-Xylene | 19.1 | 19.1 |
| 1,3,5-Trimethylbenzene | Trace | Trace |
| **Total Flow (lb/hr)** | 2104 | 2104 |
| **Design Data** | | |
| Subtype | Centrifugal | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 18.2 | |
| Head (ft) | 98.4 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$11,324.71** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| PUMP | | |
|---|---|---|
| Identification: P-302 | | |
| Function: Pumps the liquid from the bottom of the column COL-301 to the reboiler RB-301. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-306 | S-307 |
| Benzene | 174298 | 174298 |
| Toluene | 61609 | 61609 |
| P-Xylene | 13244 | 13244 |
| 1,3,5-Trimethylbenzene | 14893 | 14893 |
| **Total Flow (lb/hr)** | 264044 | 264044 |
| **Design Data** | | |
| Subtype | Centrifugal Pump | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 5.57 | |
| Head (ft) | 29.3 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$14,602.61** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| PUMP | | |
|---|---|---|
| Identification: P-303 | | |
| Function: Pumps the liquid reflux from the reflux accumulator RA-302 to the distillation column, COL-302. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-313 | S-314 |
| Benzene | 70269 | 70269 |
| Toluene | 34673 | 34673 |
| P-Xylene | 9136 | 9136 |
| 1,3,5-Trimethylbenzene | 40.5 | 40.5 |
| **Total Flow (lb/hr)** | 114118 | 114118 |
| **Design Data** | | |
| Subtype | Centrifugal Pump | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 285 | |
| Head (ft) | 83.7 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$13542.95** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| PUMP | | |
|---|---|---|
| Identification: P-304 | | |
| Function: Pumps the liquid from the bottom of the column COL-302 to the reboiler RB-302. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-316 | S-317 |
| Benzene | Trace | Trace |
| Toluene | Trace | Trace |
| P-Xylene | 404 | 404 |
| 1,3,5-Trimethylbenzene | 194050 | 194050 |
| **Total Flow (lb/hr)** | 194453 | 194453 |
| **Design Data** | | |
| Subtype | Centrifugal Pump | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 628 | |
| Head (ft) | 444 | |
| Pump Type | 3600 RPM, VSC, 40 - 500 ft, 50 - 900 gpm, 75 hp | |
| **Purchase Cost** | **$22,006.77** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| PUMP | | |
|---|---|---|
| Identification: P-401 | | |
| Function: Pumps water to the steam boiler. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-401 | S-402 |
| Water | 1015890 | 1015890 |
| **Total Flow (lb/hr)** | 1015890 | 1015890 |
| **Design Data** | | |
| Subtype | Centrifugal Pump | |
| Construction Material | Cast Iron | |
| Flow Rate (gpm) | 2040 | |
| Head (ft) | 500 | |
| Pump Type | 1800 RPM, HSC, 50 - 500 ft, 250 - 5000 gpm, 250 Hp | |
| **Purchase Cost** | **$49,893.17** | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

## Reactor

| REACTOR | | |
|---|---|---|
| Identification: R-101, R-102, R-103 | | |
| Function: Converts ethane feedstock to desired BTX product. | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-106 | S-107 |
| Hydrogen | 2758 | 18388 |
| Methane | 118810 | 162584 |
| Ethane | 389331 | 209537 |
| Ethylene | 22090 | 22090 |
| Propane | 14463 | 9027 |
| Propylene | 2774 | 2774 |
| Benzene | 18014 | 88283 |
| Toluene | 1232 | 35905 |
| P-Xylene | 27.5 | 9178 |
| 1,3,5-Trimethylbenzene | Trace | 11739 |
| **Total Flow (lb/hr)** | 569500 | 569504 |
| **Purchase Cost (for all units)** | **$165,000,000** | |
| **Costing Information Source** | **Jacobs UK Inc.** | |

## Reboilers

| REBOILER | | | | | |
|---|---|---|---|---|---|
| Identification: RB-301 | | | | | |
| Function: Uses high pressure steam to vaporize the liquid leaving the bottom of distillation column COL-301. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Hot Side | | Cold Side | | |
| | Feed 1 | Exit 1 | Feed 2 | Exit 2 | Exit 3 |
| **Materials Handled:** | S-408 | S-308 | S-307 | S-309 | S-310 |
| Benzene | 0 | 0 | 174298 | 104030 | 70269 |
| Toluene | 0 | 0 | 61609 | 26936 | 34673 |
| P-Xylene | 0 | 0 | 13244 | 4094 | 9151 |
| 1,3,5-Trimethylbenzene | 0 | 0 | 14893 | 3154 | 11739 |
| Water | 25705 | 25705 | 0 | 0 | 0 |
| **Total Flow (lb/hr)** | 25705 | 25705 | 264044 | 138214 | 125831 |
| **Design Data** | | | | | |
| Subtype | Kettle Vaporizer | | | | |
| Shell/Tube Material | Carbon Steel/Carbon Steel | | | | |
| Tube Length (ft) | 20 | | | | |
| Surface Area ($ft^2$) | 971 | | | | |
| Shell-Side Pressure (psig) | 84.5 | | | | |
| **Purchase Cost** | **$112,298.87** | | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | | |

| REBOILER | | | | | |
|---|---|---|---|---|---|
| Identification: RB-302 | | | | | |
| Function: Uses high pressure steam to vaporize the liquid leaving the bottom of distillation column COL-302. | | | | | |
| Operation: Continuous | | | | | |
| | **Mass Flow (lb/hr)** | | | | |
| | Hot Side | | Cold Side | | |
| | Feed 1 | Exit 1 | Feed 2 | Exit 2 | Exit 3 |
| **Materials Handled:** | S-409 | S-319 | S-317 | S-318 | S-320 |
| Benzene | 0 | 0 | Trace | Trace | Trace |
| Toluene | 0 | 0 | Trace | Trace | Trace |
| P-Xylene | 0 | 0 | 404 | 389 | 14.7 |
| 1,3,5-Trimethylbenzene | 0 | 0 | 194050 | 182351 | 11698 |
| Water | 31936 | 31936 | 0 | 0 | 0 |
| **Total Flow (lb/hr)** | 31936 | 31936 | 194453 | 182741 | 11713 |
| **Design Data** | | | | | |
| Subtype | Kettle Vaporizer | | | | |
| Shell/Tube Material | Carbon Steel/Carbon Steel | | | | |
| Tube Length (ft) | 20 | | | | |
| Surface Area ($ft^2$) | 488 | | | | |
| Shell-Side Pressure (psig) | 44.5 | | | | |
| **Purchase Cost** | **$90,969.10** | | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | | |

## Reflux Accumulators

| REFLUX ACCUMULATOR | | | |
|---|---|---|---|
| Identification: RA-301 | | | |
| Function: Stores reflux from top of column to maintain constant reflux and distillate flow rates. | | | |
| Operation: Continuous | | | |
| | **Mass Flow (lb/hr)** | | |
| | Feed | Exit 1 | Exit 2 |
| **Materials Handled:** | S-302 | S-303 | S-305 |
| Hydrogen | Trace | Trace | Trace |
| Methane | 2723 | 5.39 | 2717 |
| Ethane | 7089 | 50.7 | 7038 |
| Ethylene | 612 | 3.61 | 608 |
| Propane | 720 | 9.08 | 711 |
| Propylene | 144 | 1.07 | 143 |
| Benzene | 10037 | 1664 | 8373 |
| Toluene | 1186 | 351 | 835 |
| P-Xylene | 42.8 | 19.1 | 23.7 |
| 1,3,5-Trimethylbenzene | Trace | Trace | Trace |
| **Total Flow (lb/hr)** | 22553 | 2104 | 20449 |
| **Design Data** | | | |
| Length (ft) | 36.6 | | |
| Inner Diameter (ft) | 18.3 | | |
| Wall Thickness (in) | 0.625 | | |
| Operating Pressure (psig) | 10 | | |
| Vessel Material | Carbon Steel | | |
| **Purchase Cost** | **$418,852.67** | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | |

| REFLUX ACCUMULATOR | | | |
|---|---|---|---|
| Identification: RA-302 | | | |
| Function: Stores reflux from top of column to maintain constant reflux and distillate flow rates. | | | |
| Operation: Continuous | | | |
| | **Mass Flow (lb/hr)** | | |
| | Feed | Exit 1 | Exit 2 |
| **Materials Handled:** | S-312 | S-313 | S-315 |
| Benzene | 115357 | 70269 | 70269 |
| Toluene | 56920 | 34673 | 34673 |
| P-Xylene | 14998 | 9136 | 9136 |
| 1,3,5-Trimethylbenzene | 66.5 | 40.5 | 40.5 |
| **Total Flow (lb/hr)** | 187342 | 114118 | 114118 |
| **Design Data** | | | |
| Length (ft) | 14.8 | | |
| Inner Diameter (ft) | 7.41 | | |
| Wall Thickness (in) | 0.500 | | |
| Operating Pressure (psig) | 10 | | |
| Vessel Material | Carbon Steel | | |
| **Purchase Cost** | **$38,593.29** | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | |

## Storage Tanks

| STORAGE TANK | |
|---|---|
| Identification: ST-201, ST-202, ST-203 | |
| Function: Stores the BTX product. Each tank has a capacity of one day. | |
| Operation: Batch | |
| | **Mass Flow (lb/hr)** |
| | Feed |
| **Materials Handled:** | S-215 |
| Benzene | 70269 |
| Toluene | 34673 |
| P-Xylene | 9136 |
| 1,3,5-Trimethylbenzene | 40.5 |
| **Total Flow (lb/hr)** | 114118 |
| **Design Data** | |
| Storage Capacity (gal) | 590,367 |
| **Purchase Cost** | **$1,418,078.05** |
| **Costing Information Source** | **Product and Process Design Principles**[14] |

| STORAGE TANK | |
|---|---|
| Identification: ST-204, ST-205, ST-206 | |
| Function: Stores the gasoline-blend product. Each tank has a capacity of one day. | |
| Operation: Batch | |
| | **Mass Flow (lb/hr)** |
| | Feed |
| **Materials Handled:** | S-216 |
| Benzene | Trace |
| Toluene | Trace |
| P-Xylene | 14.7 |
| 1,3,5-Trimethylbenzene | 11698 |
| **Total Flow (lb/hr)** | 11713 |
| **Design Data** | |
| Storage Capacity (gal) | 40429 |
| **Purchase Cost** | **$59,246.38** |
| **Costing Information Source** | **Product and Process Design Principles**[14] |

## Turbines

| TURBINE | | |
|---|---|---|
| Identification: T-101, T-102, T-103 | | |
| Function: To recover work from permeate coming out of PRISM | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-218 | S-103 |
| Hydrogen | 2758 | 2758 |
| Methane | 115104 | 115104 |
| Ethane | 202499 | 202499 |
| Ethylene | 21482 | 21482 |
| Propane | 8316 | 8316 |
| Propylene | 2630 | 2630 |
| Benzene | 9641 | 9641 |
| Toluene | 397 | 397 |
| P-Xylene | 3.73 | 3.73 |
| 1,3,5-Trimethylbenzene | Trace | Trace |
| **Total Flow (lb/hr)** | 362832 | 362832 |
| **Design Data** | | |
| Power Extracted (hp) | 4089.8 | |
| **Purchase Cost** | $446,431.21 | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| TURBINE | | |
|---|---|---|
| Identification: T-104 | | |
| Function: To recover work from feedstock ethane | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-101 | S-102 |
| Methane | 989 | 989 |
| Ethane | 179794 | 179794 |
| Propane | 5436 | 5436 |
| **Total Flow (lb/hr)** | 186219 | 186219 |
| **Design Data** | | |
| Power Extracted (hp) | 2563.94 | |
| **Purchase Cost** | $305,837.85 | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| TURBINE | | |
|---|---|---|
| Identification: T-105 | | |
| Function: To recover work from distillate from the first distillation column’s reflux accumulator | | |
| Operation: Continuous | | |
| | **Mass Flow (lb/hr)** | |
| | Feed | Exit |
| **Materials Handled:** | S-305 | S-104 |
| Methane | 2717 | 2717 |
| Ethane | 7038 | 7038 |
| Ethylene | 608 | 608 |
| Propane | 711 | 711 |
| Propylene | 143 | 143 |
| Benzene | 8373 | 8373 |
| Toluene | 835 | 835 |
| P-Xylene | 23.7 | 23.7 |
| 1,3,5-Trimethylbenzene | Trace | Trace |
| **Total Flow (lb/hr)** | 20449 | 20449 |
| **Design Data** | | |
| Power Extracted (hp) | 95.91 | |
| **Purchase Cost** | $21,359.83 | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | |

| TURBINE | | | | |
|---|---|---|---|---|
| Identification: T-401 | | | | |
| Function: Extracts energy from the high pressure steam to a pressure that can be used for the heating requirements of the reboilers, RB-301 and RB-302, and heat exchanger, H-203. | | | | |
| Operation: Continuous | | | | |
| | **Mass Flow (lb/hr)** | | | |
| | Feed | Exit 1 | Exit 2 | Exit 3 |
| **Materials Handled:** | S-406 | S-407 | S-408 | S-409 |
| Water | 80467 | 22826 | 25705 | 31936 |
| **Total Flow (lb/hr)** | 80467 | 22826 | 25705 | 31936 |
| **Design Data** | | | | |
| Power Extracted (hp) | 1691 | | | |
| **Purchase Cost** | **$218,254.90** | | | |
| **Costing Information Source** | **Product and Process Design Principles**[14] | | | |

# Equipment Cost Summary

Table 31. Cost and source of each unit of equipment. Pricing sources for equipment that was not priced with Product and Process Design Principles may be found in Appendix A-6.

| ID | Description | Price Source | Cost |
|---|---|---|---|
| COND-301 | Condenser | Product and Process Design Principles[14] | $64,974.99 |
| COND-302 | Condenser | Product and Process Design Principles[14] | $198,069.53 |
| | | | |
| C-201 | Multistage Compressor | Product and Process Design Principles[14] | $16,068,647.94 |
| C-202 | Multistage Compressor | Product and Process Design Principles[14] | $16,068,647.94 |
| | | | |
| COL-201 | Flash Drum | Product and Process Design Principles[14] | $496,260.10 |
| | | | |
| COL-301 | Distillation Column | Product and Process Design Principles[14] | $946,959.53 |
| COL-302 | Distillation Column | Product and Process Design Principles[14] | $1,422,606.78 |
| | | | |
| F-401 | Fired Heater | Consultant Provided | $10,682,210.00 |
| | | | |
| H-201 | Heat Exchanger | Product and Process Design Principles[14] | $78,762.43 |
| H-202 | Heat Exchanger | Product and Process Design Principles[14] | $68,821.01 |
| H-203 | Heat Exchanger | Product and Process Design Principles[14] | $80,482.61 |
| | | | |
| P-101 | Centrifugal Pump | Product and Process Design Principles[14] | $15,500.06 |
| P-201 | Centrifugal Pump | Product and Process Design Principles[14] | $10,854.43 |
| P-202 | Centrifugal Pump | Product and Process Design Principles[14] | $10,818.20 |
| P-301 | Centrifugal Pump | Product and Process Design Principles[14] | $9,747.16 |
| P-302 | Centrifugal Pump | Product and Process Design Principles[14] | $12,877.08 |
| P-303 | Centrifugal Pump | Product and Process Design Principles[14] | $13,542.95 |
| P-304 | Centrifugal Pump | Product and Process Design Principles[14] | $12,990.48 |
| P-401 | Centrifugal Pump | Product and Process Design Principles[14] | $49,893.17 |
| | | | |
| PR-201 | PRISM | Air Products and Chemicals, Inc. | $17,000,000.00 |
| | | | |
| R-101 | Steam Reformer Reactor | Jacobs UK | $55,000,000.00 |

| ID | Description | Price Source | Cost |
|---|---|---|---|
| R-102 | Steam Reformer Reactor | Jacobs UK | $55,000,000.00 |
| R-103 | Steam Reformer Reactor | Jacobs UK | $55,000,000.00 |
| | | | |
| RB-301 | Reboiler | Product and Process Design Principles[14] | $148,379.15 |
| RB-302 | Reboiler | Product and Process Design Principles[14] | $107,486.22 |
| | | | |
| RA-301 | Reflux Accumulator | Product and Process Design Principles[14] | $663,053.24 |
| RA-302 | Reflux Accumulator | Product and Process Design Principles[14] | $133,482.62 |
| | | | |
| T-101 | Power-Recovery Turbine | Product and Process Design Principles[14] | $506,252.99 |
| T-102 | Power-Recovery Turbine | Product and Process Design Principles[14] | $506,252.99 |
| T-103 | Power-Recovery Turbine | Product and Process Design Principles[14] | $506,252.99 |
| T-104 | Power-Recovery Turbine | Product and Process Design Principles[14] | $346,820.12 |
| T-105 | Power-Recovery Turbine | Product and Process Design Principles[14] | $24,222.05 |
| T-401 | Power-Recovery Turbine | Product and Process Design Principles[14] | $220,567.45 |
| | | | |
| ST-201 | Storage Tank | Product and Process Design Principles[14] | $472,692.68 |
| ST-202 | Storage Tank | Product and Process Design Principles[14] | $472,692.68 |
| ST-203 | Storage Tank | Product and Process Design Principles[14] | $472,692.68 |
| ST-204 | Storage Tank | Product and Process Design Principles[14] | $82,619.28 |
| ST-205 | Storage Tank | Product and Process Design Principles[14] | $82,619.28 |
| ST-206 | Storage Tank | Product and Process Design Principles[14] | $82,619.28 |
| | | | |
| PV-101 | Pressure Vessel | Product and Process Design Principles[14] | $1,441,023.07 |

## Fixed-Capital Investment Summary

The total fixed costs were calculated from the total cost of operations, maintenance, operating overhead, property insurance, and taxes. The total fixed cost was calculated as $12.7MM. Table 32 summaries the fixed-capital investment breakdown.

Table 32. Fixed-capital investment breakdown.

| **Operations** | **Annual Cost** |
|---|---|
| Direct Wages and Benefits | $3,328,000 |
| Direct Salaries and Benefits | $499,200 |
| Operating Supplies and Services | $199,680 |
| Technical Assistance to Manufacturing | $2,400,000 |
| Control Laboratory | $2,600,000 |
| **Total Operations** | **$9,026,880** |
| | |
| **Maintenance** | **Annual Cost** |
| Wages and Benefits | $10,616,126 |
| Salaries and Benefits | $2,654,032 |
| Materials and Services | $10,616,126 |
| Maintenance Overhead | $530,806 |
| **Total Maintenance** | **$24,417,091** |
| | |
| **Operating Overhead** | **Annual Cost** |
| General Plant Overhead: | $1,213,912 |
| Mechanical Department Services: | $410,337 |
| Employee Relations Department: | $1,008,744 |
| Business Services: | $1,265,204 |
| **Total Operating Overhead** | **$3,898,198** |
| | |
| **Property Taxes and Insurance** | **Annual Cost** |

| | |
|---|---:|
| Property Taxes and Insurance: | $6,066,358 |
| | |
| **Total Fixed Costs** | **$43,408,526** |

Guidelines provided in Chapter 23 of Product and Process Design Principles[14] were used to arrive at these numbers. Eight operators will operate this plant per shift. This number was calculated by multiplying four operators (one for each process section) by a factor of two since this plant is a continuous-flow process that produces over 1,000 tons of products per day. Direct wages and benefits (DW&B) are assumed at $40 per operator-hour. In addition, costs for direct salaries and benefits for supervisory and engineering personnel is set at 15% of DW&B and operating supplies and services is set at 6% of DW&B. Finally, $60,000 per operator-shift-year is added for technical assistance and $65,000 per operator-shift-year for the control laboratory. Wages and benefits for maintenance staff (MW&B) is set at 3.5% of total depreciable capital (TDC), since this process deals with fluids only. Costs of maintenance staff wages and benefits, materials and services, and maintenance overhead are estimated at 25%, 100%, and 5% of MW&B costs respectively. Furthermore, general plant overhead was set at 7.1% of maintenance and operations wages and benefits (MOW&B). Costs of mechanical department services, employee relations, and business services are set at 2.4%, 5.9%, and 7.4%, respectively. Finally, property taxes and property insurance costs were estimated at 2% of TDC. Since this process is located on a fairly large plant, this analysis did not take into account any additional costs such as rental fees and licensing fees.

# Operating Cost - Cost of Manufacture

Table 33. Variable cost breakdown.

| | | | |
|---|---|---|---|
| **Variable Costs at 100% Capacity:** | | | |
| | | | |
| **General Expenses** | | | |
| Selling / Transfer Expenses: | | | $11,198,277 |
| Direct Research: | | | $17,917,244 |
| Allocated Research: | | | $1,866,380 |
| Administrative Expense: | | | $7,465,518 |
| Management Incentive Compensation: | | | $4,665,949 |
| | | | |
| **Total General Expenses** | | | $43,113,367 |
| | | | |
| **Raw Materials** | $0.341 | per lb of BTX | $318,535,578 |
| **Byproducts** | $0.113 | per lb of BTX | ($102,397,305) |
| **Utilities** | $0.030 | per lb of BTX | $27,762,245 |
| | | | |
| **Total Variable Costs** | | | **$287,013,885** |

## Profitability Analysis - Business Case

The return on investment is calculated as the ratio of net annual earnings, including income tax and a five-year MACRS depreciation schedule, and the total capital investment, adjusted for working capital effects. This process has an ROI of -0.94% based on the third production year.

Table 34. ROI Analysis (Third Production Year)

| | |
|---|---|
| Annual Sales | $288,418,629 |
| Annual Costs | $(266,487,209) |
| Depreciation | $(27,177,283) |
| Income Tax | $1,940,969 |
| Net Earnings | $(3,304,894) |
| Total Capital Investment | $351,308,449 |
| **ROI** | **-0.94%** |

The Internal Rate of Return (IRR) for this project is 2.87% and the Net Present Value (NPV) for the project is -$166,765,000 at a discount rate of 18%. These values were calculated using the "Profitability Analysis" Excel worksheet introduced as part of the Product and Process Design Principles[14]. The full spreadsheet is attached in Appendix A-3: Profitability Analysis Reports. Looking at these numbers, it is evident that the plant is currently an economically unfavorable business venture. The most important variables that contribute to profitability are primary input (ethane) costs, catalyst component costs (primarily platinum and zeolite), and catalyst lifespan. Other important factors that lead to this high internal rate of return have been addressed in the following sections. These factors include the price of nitrogen, price of BTX as the main product, and fixed and variable costs.

## Overall Revenue and Cost Analysis

*Revenue Analysis*

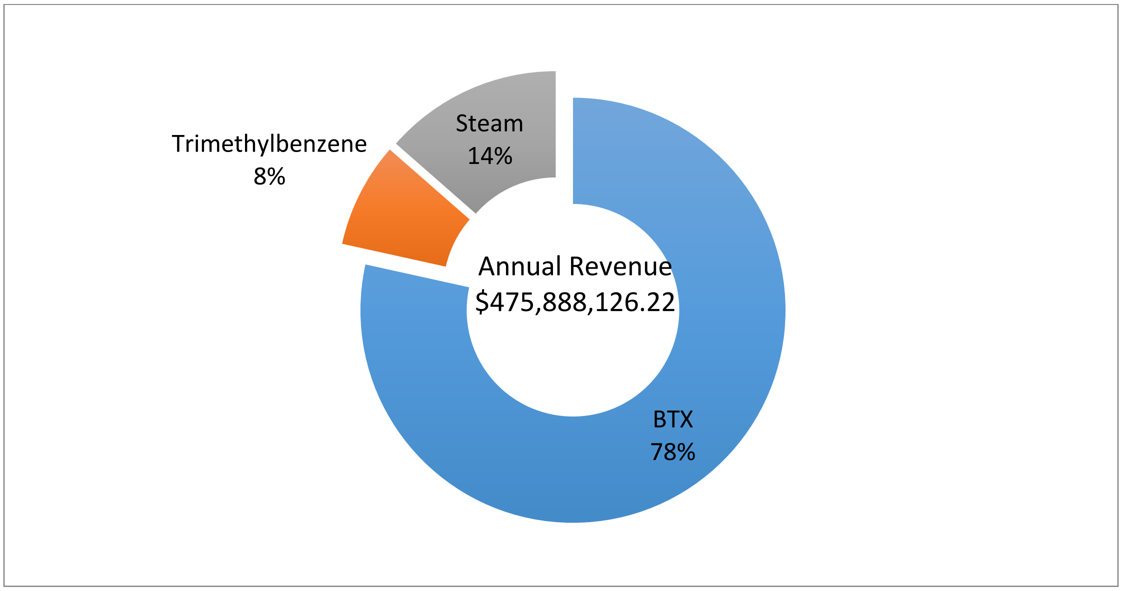


Figure 10. Revenue Stream Analysis

Analysis on the revenue stream was conducted to examine the source of revenue of the project and is presented in Figure 10. As expected, BTX accounts for 78% of the entire revenue stream and trimethylbenzene accounts for 8%. Surprisingly, the revenue generated from selling excess steam created during the process brings in a greater proportion of revenue than trimethylbenzene.

*Cost Analysis*

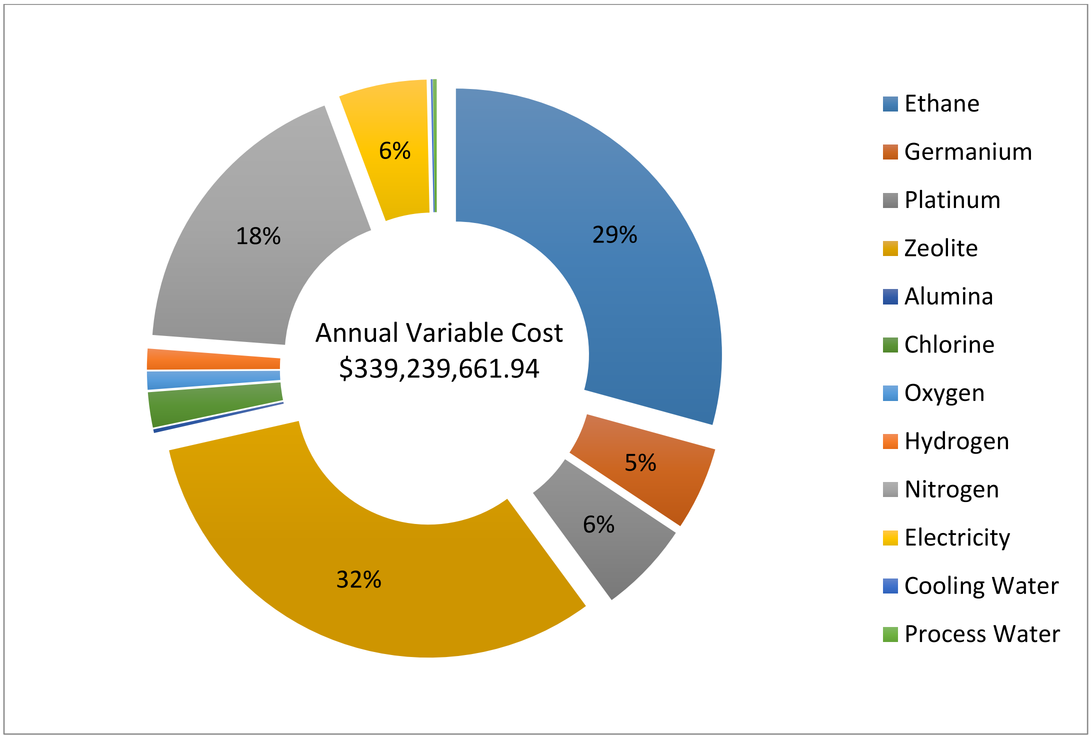


Figure 11. Variable Cost Analysis

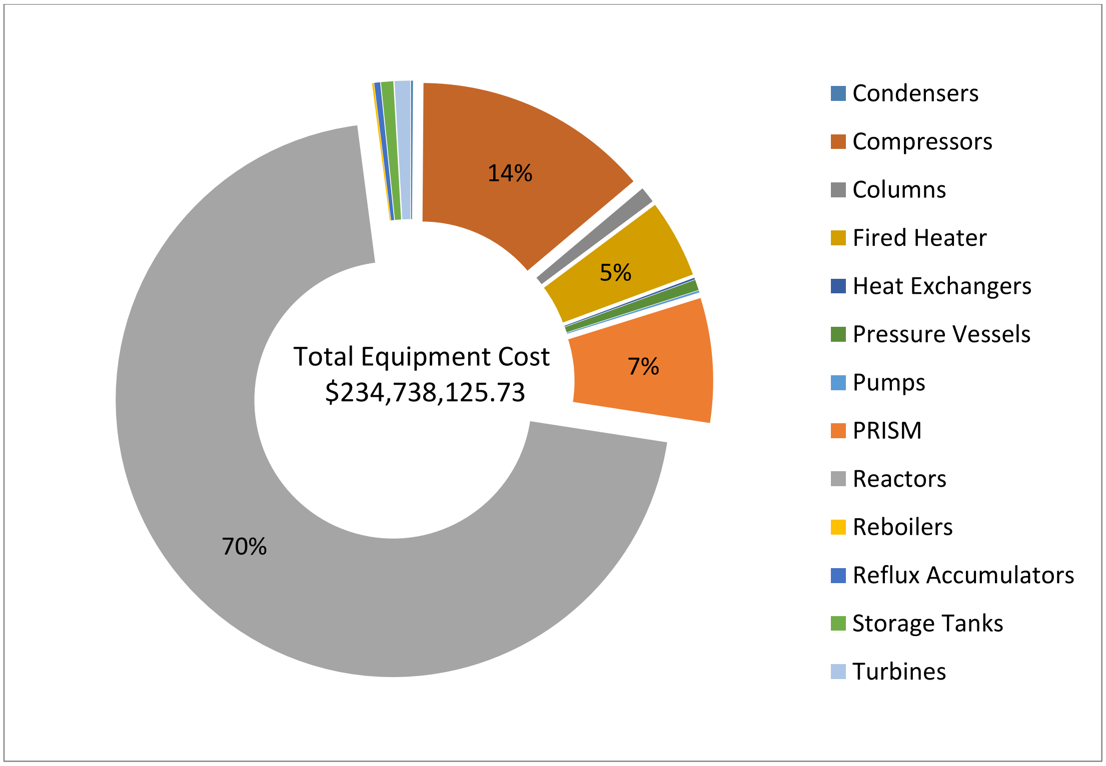


Figure 12. Equipment Cost Analysis

Analysis on the cost streams was conducted on variable and equipment costs. As shown in Figure 11 above, 42% of the variable cost consisted of catalyst costs. An additional 29% was contributed by the cost of the main feedstock ethane. Regeneration chemicals nitrogen, chlorine, hydrogen, and oxygen added 22%. Conversely, utilities contributed only 5% of total variable costs. Thus, the IRR and NPV for the project depend very much on catalyst and ethane prices, which will be shown in the Sensitivity Analyses section below. Meanwhile, the three reactors required for the plant constitute 70% of equipment costs. The PRISM separation membrane, multistage compressor, and fired heater contribute an additional 26% of the total costs, such that these six pieces of equipment make up almost the entirety of the cost of manufacture.

## Sensitivity Analyses

*Sensitivity Analysis on Feed Price*

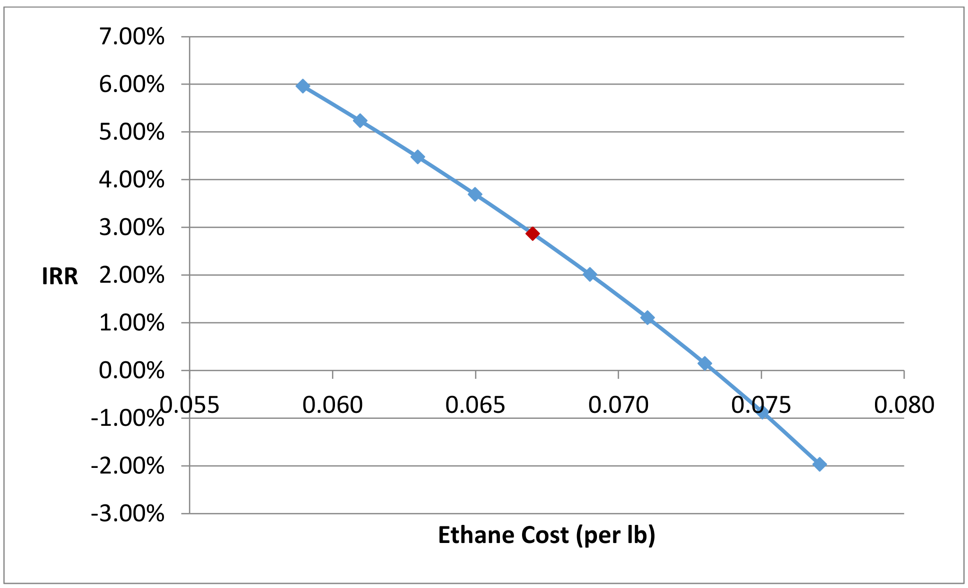


Figure 13. Effect of Ethane Price on IRR

With an estimated price of ethane of $0.067 per lb, the IRR is 2.87%. The IRR of the project is fairly sensitive to the price of ethane, as it is the only feedstock into the process. Sensitivity analysis was conducted on ethane price on an increase/decrease of up to 15%. Historical prices for ethane have been fairly stable, as exhibited in Figure 4, thus a limited range of volatility was chosen. As shown in Figure 13, the IRR remains positive within most of this range of prices. Further, it is unlikely that ethane's cost would be higher than this range, since the estimate comes from current market spot prices. In reality, the feed of ethane is actually fractional grade ethane coming as a waste product from other hydrocarbon processing plants in the Gulf Coast, which is not pure ethane and would likely be cheaper than our estimates. Thus, in the event overall natural gas prices fall significantly, the price of ethane would likely follow suit, and greatly increase the IRR.

*Sensitivity Analysis on Product Price*

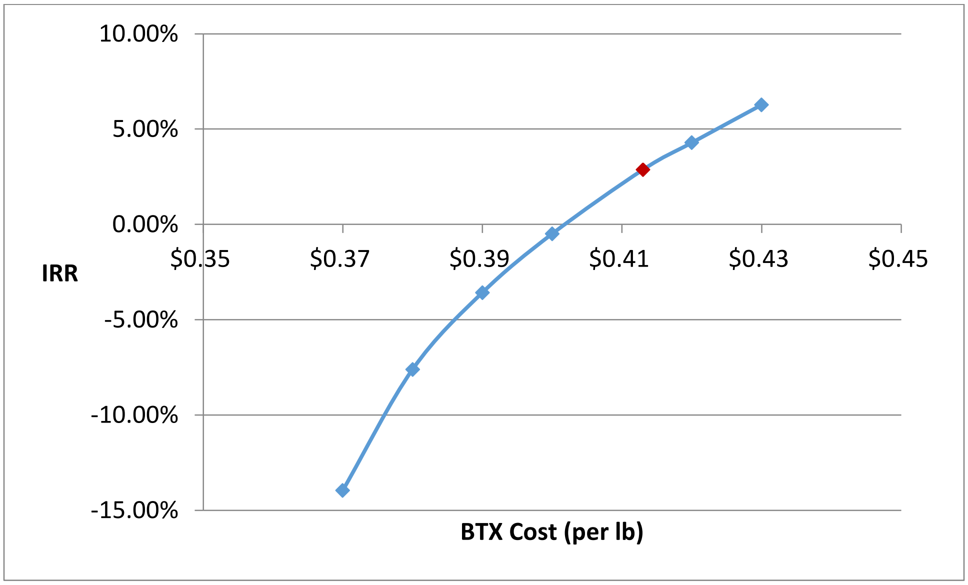


Figure 14. Effect of BTX price on IRR

As seen in Figure 10 in the revenue stream analysis, 78% of the revenue comes from BTX, which is the main product from the process. A sensitivity analysis was conducted on the selling price of BTX, as the profitability of the project is heavily dependent on it. As stated in the problem statement for this project, BTX prices have been fairly stable at $3.00 per gallon, or $0.413 per lb. As expected, the IRR increases as the price of BTX increases. However, the project can maintain a positive IRR only in market conditions where the price of BTX stays above $0.40 per lb, a level that can be tested by a drop in crude oil prices.

*Sensitivity Analysis on Catalyst Cost*


Figure 15. Effect of zeolite price on IRR

As 77% of the variable cost, the catalyst and its components greatly influence the profitability of the project. At 57% of total variable cost, zeolite is the costliest of the components, and thus a sensitivity analysis was conducted on the price of zeolite. At a price of $12.50 per kg, the IRR is 2.87%. Due to disagreeing estimates of the cost of $5/kg and $15/kg, a range of prices between the two were considered. In order to retain a positive IRR, the zeolite price can be no greater than $13.50 per kg. This calculates to an 8% premium on the current estimated price, a small but not insignificant. The low estimate of $5/kg would meet an IRR of 16.10%.

*Sensitivity Analysis on Catalyst Lifetime*

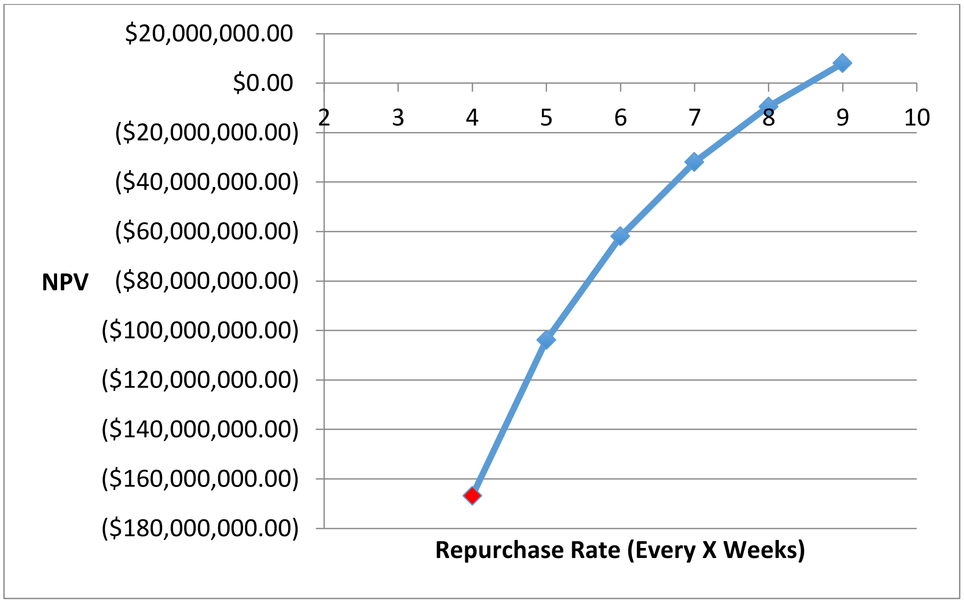


Figure 16. Effect of catalyst lifetime on NPV

For the same reasons stated under Sensitivity Analysis on Catalyst Cost, a sensitivity analysis was conducted on catalyst lifetime. An increase in the expected lifetime of the catalyst would lead to less frequent repurchases of the catalyst components, and hence lower costs. Figure 16 shows the effect of the catalyst lifetime on NPV, and one can see that an increase of just a few weeks in lifetime puts the NPV into positive territory. The current estimate of a lifetime of four weeks or one month is already a conservative estimate for catalyst lifetimes in industrial processes, so we see potential for the project will to become profitable. However, due to the sensitivity of NPV to changes in the catalyst lifetime, every step should be taken to maximize the lifetime of the catalyst. A one-month increase in the catalyst lifetime from one to two months increases the NPV by over $150 million.

## Assumptions for Economic Analysis

**Tax rate:** 37%

**Cost of capital:** 18%. Due to the presumed mature nature of the Company, a discount rate in the range of 10-25% was chosen[25].

**Tax Credit:** In economic analysis, the Company was assumed to be profitable during the lifetime of plant operation, and therefore the Company holds no tax credits or carryover losses.

**Operating Times:** The plant was assumed to operate 330 days a year for 24 hours a day. First year production was also assumed to be 50% of full production capacity, with a linear ramp-up over three years to 90% of full capacity in the third year and onwards.

**Salvage Value:** Given the highly specific nature of the equipment and a long operating period of 15 years, there was assumed to be no salvage value to the plant.

# Other Important Considerations

## Safety

Almost all streams and equipment in this process operate at high pressures and temperatures. Also, the hydrocarbons in this process are volatile and flammable. All operators and employees on the plant should be equipped with safety equipment, well trained on safety procedures if a disaster should arise and be cognizant of the normal operating conditions of all equipment on the plant. Leaks should be reported immediately and all units should be inspected regularly for preventative maintenance. All chemicals should be handled with care and copies of the Material Safety Data Sheets (MSDS) that are located in Appendix A-4 should be made available to all employees.

## Maintenance

The process design allows the plant to be continuously operational for 330 days in a year, with the remainder reserved for maintenance. For the reactors (R-101, R-102, and R-103), the spent catalyst will be replaced monthly. The heat exchangers will have to be cleaned and inspected for fouling for improved heat transfer. In addition, condensers and reboilers should be inspected for fouling and corrosion.

The turbines will need to have motors and pumps replaced in case of failure.[22] The storage tanks and pressure vessel should be cleaned of leftover product, sludge, and solids built up throughout the 330 day cycle. Whenever a primary pump in the process fails, the safety pump should be operational and workers should identify whether the primary pump can be fixed or if a new pump will have to be purchased. Distillation columns[23] and flash vessels are associated with failure modes such as overheating, impurities, and leaks[6]. This could potentially lead to weekly maintenance checks on these pieces of equipment due to the large amount of material passing through them. For the steam boilers, failures in the fan should be avoided to ensure that enough steam utility is supplied for the process[8]. Lastly, the PRISM unit will need to be checked regularly due to its high operating conditions and large feed flow rates.

## Startup

The cost of plant startup will be close to 10% of the total depreciable capital cost[13]. Due to the large amounts of chemicals being processed and the size of the equipment being considered, enough time must be taken to achieve steady state in the major pieces of equipment (e.g., reactor, distillation columns) before production can begin. The startup plan must account for additional pieces of equipment, such as heat exchangers, which will assist in achieving appropriate temperatures for safe operation. Safe methods for the transport of feedstock, product, and other key chemicals will also be required; the costs of setting up pipelines to ferry ethane feedstock and hydrogen to the site must be included, as well as the costs of transporting the final BTX product to an adjacent plant for use.

## Environmental

This process consumes a significant amount of energy that is produced through the burning of fuel gas (a mixture of hydrogen, methane, C2, and C3-hydrocarbons). Therefore the process will produce significant $NO_x$ and $CO_2$ emissions, which will require government permits in order to follow federal and state regulations. In addition, the gaseous chemicals involved in the regeneration cost may need to be scrubbed before release into the atmosphere.

## Control

The implementation of flow-control valves is necessary to reduce disturbances and keep the process under a strict, continuous schedule. The flow control valves should operate either with proportional-integral or proportional-integral-derivative control. All flow control valves contacted with streams below 900°F can be constructed with carbon steel[24]; otherwise, stainless steel AISI 304L can be used for temperatures below 1400°F. A type of control valve to consider is the single-port valve body due to its frequent usage in industrial plants[8].

Flow control valves should be used for the multistage compressors C-201 and C-202 to keep the compressors below an electricity requirement of 30,000 hp. For storage tanks ST-201 through ST-206, the BTX and heavy hydrocarbon products will have a valve corresponding to each storage tank to ensure that products are evenly distributed. For condensers COND-301 and COND-302, valves should be put for the cooling water utilities to adjust for disturbances in the tube side inlet temperatures. Similarly, for reboilers RB-301 and RB-302, valves should be placed on the steam utilities to adjust for disturbances in the shell side inlet temperatures. For the reactor inlet stream, S-106, a valve should be implemented to adjust for a higher or lower expected amount of material from the recycle streams. In addition, there should be three valves to ensure that flow does not go through a reactor undergoing regeneration. Lastly, the pipelines containing the materials used in the regeneration process should each have a valve to adjust the amount of material going into a reactor with respect to regeneration stage.

## Pilot Plant

Several assumptions have been made in this preliminary analysis that will need to be tested in a pilot plant before proceeding to full industrial scale. As the catalyst is novel and has not yet been used industrially, it will need to be tested to determine whether there are significant changes to conversion and selectivity data when scaling up from laboratory experiments. Another key assumption is the lifetime of the catalyst: the patent authors performed short single pass conversion tests that did not account for deactivation. At the current harsh operating conditions of the reactor, coke formation will certainly foul the catalyst surface, and the costs of the catalyst itself and of the regeneration process depend on the number of times the catalyst can be regenerated and replaced. Significant deactivation of catalyst would lead to higher operating costs, increasing the length of time to achieve profitability.

## Conclusions and Recommendations

After a meticulous analysis of materials, utilities, equipment, and profitability of the process, we have concluded that the process will be unprofitable under the internal rate of return criterion of 15%. The total capital cost of the process is $347,191,577 and the operating cost is $287,013,885 per year. Overall, the IRR for this project is estimated as 2.87% and the NPV is estimated at -$166,765,000 at a discount rate of 18%.

Due to the plentiful supply of raw materials and to the availability of consumers of BTX and other side products in the area, the Gulf Coast is the optimal location for this plant. The main factors that affect the IRR are the cost of ethane, cost of catalyst material, and the catalyst lifespan. Under sensitivity analysis of our inputs, we find that in order for this project to be profitable, the repurchase rate/lifetime of our catalyst needs to be 8.5 weeks or longer. Alternatively, a zeolite price of under $5.50 per kg would return an IRR of over 15%. In addition, a rise in the price of BTX to $0.47 per lb will also yield an IRR value of over 15%. Further, there are concerns surrounding price stability due to the recent drop in crude oil and natural gas prices. Therefore, this process should only be carried out under particular advantageous market conditions.

Multiple assumptions made through this process design will need to be investigated to improve the profitability of this project. The transition from experimental- to industrial-scale production must be carefully observed over a suggested span of one month to evaluate any failures in the process equipment and to determine effects of scale-up on conversions. In particular, the effects of scale-up on the lifetime of the catalyst must be examined in detail, as no information was provided in the patent. In addition, the regeneration process should undergo further research to reduce the time and amount of material required per stage. Methods to reduce or eliminate hydrogen and methane should be developed to reduce the cost of separation and compression utilities. Process equipment with large flow rates such as the PRISM unit will need careful maintenance to prevent buildup of excess methane and hydrogen.

Based on the economic analyses and recommendations stated above, construction of the proposed plant to produce 0.5MM tons of BTX per year is not recommended. The IRR of 2.87% and the negative NPV of $167 million, along with a trend of decreasing price of natural gas and of BTX, are the important considerations supporting this recommendation.

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# Appendices

## A-1. Problem Statement

**BTX from Ethane**
**(recommended by Richard Bockrath, Consultant – formerly DuPont)**

**Background.** The recent explosion of fracking in the USA is dramatically increasing the availability of light paraffinic hydrocarbons for use as feedstocks. This is especially true for ethane. Numerous olefin cracker projects have recently been announced along the Gulf Coast using ethane as the feedstock. Your company is a major consumer of BTX for plastics and other downstream products and your management has asked your team to evaluate the feasibility of using ethane as a feedstock to make BTX. You are to view this as a preliminary analysis. If your analysis is promising, more resources will be added to address the uncertainties you will likely uncover to flesh out a detailed proposal.

**Current Situation.** Alkanes-to-aromatic processes were a significant research area in the early 90s (Cyclar, Aromax, etc), but research has been less active since then – possibly due to the inability to find suitable catalysts. Your team has uncovered a recent patent by Sabic, which has a potentially novel catalyst for this application. It shows several propane-to-BTX examples. While ethane may behave differently than propane, it is about 1/6 the price of propane and more stable in pricing. Your management would like you to evaluate the patent by assuming ethane and propane will give the same conversions and selectivities. Obviously this is a key uncertainty for a future team to study if the economics look promising.

The best candidate catalyst contains germanium, which you have never seen used in a petrochemical catalyst. You will need to understand the germanium market to determine whether this catalyst is commercially viable.

When locating your plant, consider feedstock availability and the cost of transporting a liquid product(s). You are a global BTX producer with customer plants along the Gulf Coast, in the Rotterdam area, and in Shanghai. Your largest downstream customers are in the USA and Mainland China, where much of the TPA from para-xylene is consumed.

Since your team will likely lead the next phase of this analysis, clearly document your key assumptions for management. You don't want them to be surprised by your omissions!

The US Government maintains pricing information for major hydrocarbon feedstocks. A recent price for ethane appears to be stable-to-declining at \$0.25/gal.
(http://www.eia.gov/todayinenergy/detail.cfm?id=12291).

Your supply-chain experts predict that BTX will sell for an average of \$3.00/gal in the foreseeable future.

# A-2. Sample Calculations

## *A-2.1. Area of a Heat Exchanger*

The methods for calculating the area of a heat exchanger is based on methods in Chapter 18 in Process and Product Design Principles, 4th ed. Heat exchanger H-201 will be the basis of our sample calculation, which involves transferring heat for the vapor product of COL-201 and the distillate product of COL-302. An overall heat exchanger coefficient, U, is assumed to be 149.7 BTU/hr-ft$^2$-$^o$F due to the transferring of heat between vapor and liquid streams. Temperatures of each stream and the heat duty were calculated using ASPEN PLUS:

*For counter-current flow:*

$T_{hot,in}$ = 200.2$^o$F

$T_{hot,out}$ = 136.4$^o$F

$T_{cold,in}$=104.0$^o$F

$T_{cold,out}$=116.1$^o$F

Q = 3497690 BTU/hr

*Calculation of Log Mean Temperature Difference:*

$$\Delta T_1 = T_{hot,in} - T_{cold,out} = 200.2°\text{F} - 116.1°\text{F} = 84.1°\text{F}$$

$$\Delta T_2 = T_{hot,out} - T_{cold,in} = 136.4°\text{F} - 104.0°\text{F} = 32.4°\text{F}$$

$$\Delta T_{lm} = \frac{(\Delta T_1 - \Delta T_2)}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} = \frac{(84.1°\text{F} - 32.4°\text{F})}{\ln\left(\frac{84.1°\text{F}}{32.4°\text{F}}\right)} = 54.2°\text{F}$$

*Calculation of area:*

$$A = \frac{Q}{U * \Delta T_{lm}} = \frac{3497690\ \text{BTU/hr}}{(149.7\frac{\text{BTU}}{\text{hr} - \text{ft}^2 - {}^o\text{F}} * 54.2°\text{F})} = 431.1\ ft^2$$

## *A-2.2. Reactor Volume*

The weight of catalyst required depends on the volume in which reaction takes place. The gas hourly space velocity (GHSV) was specified in US Patent 209,795 as 1000 h$^{-1}$. The flow rate of the inlet to the reactor was obtained from the ASPEN stream report as 9.15*10$^6$ ft$^3$/h. Reactor volume was then calculated as follows:

$$Reactor\ volume\ [ft^3] = \frac{Inlet\ flow\ rate}{GHSV} = \frac{9.15 * 10^6 \frac{ft^3}{h}}{1000\ h^{-1}} = 9150\ ft^3$$

### *A-2.3. Catalyst Weight*

The total weight of catalyst required was calculated using a bulk density of H-ZSM-5 zeolite catalyst of 1.06 $g/cm^3$, or 66.0 $lb/ft^3$. The catalyst weight was calculated as follows:

$$Catalyst\ weight\ [lb] = (Bulk\ density) * (Reactor\ volume) = 66.0\ \frac{lb}{ft^3} * 9150\ ft^3 = 604{,}000\ lb$$

### *A-2.4. Dimensions of a Distillation Column*

The diameter of the flash vessel, COL-201, distillation columns COL-301 and COL-302 were calculated by using the correlations found in Seider et al[13].

**Notation**

| **Symbol** | **Description** |
|---|---|
| $A_a$ | Active area on tray |
| $A_h$ | Total hole area |
| $C_{SB}$ | Parameter related to a correlation based on commercial-size towers covering tray spacing from 6 to 36 inches. |
| $D_t$ | Diameter of column |
| $F_F$ | Foaming factor |
| $F_{HA}$ | Hole-area factor |
| $F_{LG}$ | Flow ratio parameter |
| $F_{ST}$ | Surface tension factor |
| H | Height of the column |
| $H_{head\ space}$ | Height of the head Space |
| $H_{sump}$ | Height of the Sump Space |
| $H_{tray}$ | Height of a single tray |
| L | Liquid mass flow rate |
| $N_{trays}$ | Number of trays |
| $T_c$ | Critical Temperature |
| $T_r$ | Reduced Temperature |
| U | Velocity of a droplet in the column |
| $U_f$ | Flooding Velocity |
| V | Vapor mass flow rate |

| | |
|---|---|
| $x_L$ | Mass fraction of liquid |
| $\rho_L$ | Density of the liquid |
| $\rho_V$ | Density of the vapor |
| $\sigma$ | Surface Tension |

Using ASPEN stream report and block report, located in Appendix A-5, for data on COL-302.

$$H = H_{head\ space} + \left(N_{trays} - 1\right) \times H_{tray} + H_{sump} \quad (1)$$

Using $H_{head\ space}$ = 4 ft, $N_{trays}$ = 42, $H_{tray}$ = 1.5 ft, $H_{sump}$ = 10 ft:

H = 77 ft

Assuming

$$U = 0.85U_f \quad (2)$$

$U_f$ may be calculated by using equation 3.

$$U_f = C_{SB}F_{ST}F_FF_{HA}\left(\frac{\rho_L-\rho_V}{\rho_V}\right)^{\frac{1}{2}} \quad (3)$$

$C_{SB}$, $F_{ST}$, $F_F$ and $F_{HA}$ must be found before the flooding velocity can be calculated.

$F_{ST}$ can be calculated using Equation 4.

$$F_{ST} = \left(\frac{\sigma}{20}\right)^{0.5} \quad (4)$$

$\sigma$ may be found by using Equation 5.

$$\sigma = 71.815 \times (1 - T_r)^{1.2362} \quad (5)$$

The average critical temperature was calculated for the liquid on stage 2 by using equation 6:

$$T_{c,avg} = \sum_i x_{L,i}T_{c,i} \quad (6)$$

$T_{c,avg}$ was determined to be 1013 R.

The temperature on the second stage was found to be 617 R. The reduced temperature was calculated using Equation 7:

$$T_{r,avg} = \frac{T}{T_{c,avg}} \quad (7)$$

$T_{r,avg}$ was found to be 0.609.

$\sigma$ was then found to be 22.5 dynes/cm by substituting $T_{r,avg}$ in equation 5.

$F_{ST}$ was then found to be 1.02 by substituting $\sigma$ into equation 4.

$C_{SB}$ may be found by finding $F_{LG}$, and the plate spacing and then using Figure 19.4 in Seider et al.

$F_{LG}$ may be found by using equation 8.

$$F_{LG} = \left(\frac{L}{V}\right) \times \left(\frac{\rho_V}{\rho_L}\right)^{0.5} \quad (8)$$

From the ASPEN Block Report, L was found to be 0.637 lb/s and V was found to be 6.74 lb/s. A stream was created of the same composition as the liquid and vapor on the second stage of the column and the densities were found to be 48.8 lb/ft$^3$ and 0.932 lb/ft$^3$ respectively.

$F_{LG}$ was then found to be 0.0131. The corresponding $C_{SB}$ value for 1.5 ft spacing was found to be 0.3 ft/s.

$F_F$ was assumed to be 1 since the contents of the column were a non-foaming system.

$F_{HA}$ was also 1 as it was assumed that $\frac{A_h}{A_a}$ = 0.1.

Substituting these values into equation 3 gives a $U_f$ of 2.2 ft/s and a U of 1.87 ft/s.

Finally the diameter may be calculated using equation 9:

$$D_t = \frac{4}{\pi} \times \frac{V}{\left(1 - \frac{A_h}{A_a}\right) U \rho_V} \quad (9)$$

The diameter of the column was found to be 2.33 ft.

## *A-2.5. Flow Rates for Regeneration Process*

**Notation**

| **Symbol** | **Description** |
|---|---|
| $m_{coke}$ | Mass of coke built up on the catalyst surface |
| $m_{catalyst}$ | Mass of the catalyst |
| $n_{coke}$ | Number of moles of coke built up on the catalyst suface |
| $n_{O2}$ | Number of moles of oxygen required to react with all the coke on the surface of the catalyst |
| $\dot{n}_{j,i}$ | Molar flow rate of component i on stage j |
| $y_{j,i}$ | Mole fraction of compound i on stage j |

Assuming that the catalyst must be regenerated when the coke deposited on the surface is 5% of its weight and all of the coke must be burned off to be regenerated.

$$m_{coke} = 0.05 m_{catalyst} \quad (10)$$

Using a value of 1.29E+06 lb, the mass of coke, $m_c$, on the surface was calculated to be 6.47E+05 lb.

The number of moles of coke, $n_{coke,}$ was then calculated by using its molecule weight and was found to be 5390 lb-mol.

By using Equation 11, the number of moles of oxygen required may be calculated.

$$C + O_2 \rightarrow CO_2 \quad (11)$$

The number of moles of oxygen, $n_{O2}$, was found to be 5390 lb-mol. Since all of the carbon was burned off after stage 2, it was assumed that an equal amount of coke was burned off in each stage. Therefore, each stage required 2695 lb-mol of oxygen was required for each stage. The flow rate of oxygen was then found by dividing by the time duration of the stage. Since stage 1 is conducted for 24 hours, the flow rate of oxygen required was found to be 112 lb-mol/hr.

The partial pressures listed for stage 1 from the patent were then used to determine the mole fraction of each gas by using Dalton's Law of Partial Pressures. The flow rate of each gas could then be calculated by using Equation 12.

$$\dot{n}_{1,i} = \dot{n}_{1,O_2} \times \frac{y_{1,i}}{y_{1,O_2}} \quad (12)$$

The flow rates of the other reagents are listed in Table 35.

Table 35. Mole fractions and flow rates required for stage 1 for each species in the regeneration process.

| **Species** | **Mole Fraction** | **Flow Rate Required for Stage 1 (lb-mol/hr)** |
|---|---|---|
| Chlorine | 0.004 | 11.2 |
| Water Vapor | 0.033 | 89.6 |
| Oxygen | 0.042 | 112 |
| Hydrogen | 0.000 | 0 |
| Nitrogen | 0.921 | 2475 |

The total flow rate of stage 1 can be found by setting $y_{1,i}$ to 1. The total flow was found to be 2688 lb-mol/hr.

Since the pressure and temperature of each stage were the same, it was assumed that the flow rate of each stage was the same. The mole flow rate of each component could then be calculated by using the mole fraction and the total mole flow rate as shown in Equation 13.

$$\dot{n}_{j,i} = \dot{n}_1 \times y_{j,i} \quad (13)$$

## A-3. Profitability Analysis Spreadsheet

# INTRODUCTION

Prepared by Brian K. Downey, Equity Research - US Royal Gas Exploration / Production, Sanford C. Bernstein & Co., LLC

This Introduction provides brief guidlines for using the Profitability Analysis 4.0. Further and extensive details about each tab are provided in Section 17.8 of the textbook (4th Edition)

You cannot enter values in the green tabs. However, you can enter values in the the other tabs, although not in every cell. This is to prevent undesired edits from the user.

Different parameters can be entered for the evaluation of the project. One can also use parameters mentioned in Table 17.1. Equipment costs can be generated from APEA or the equations in Chapter 16 of the textbook. These two methods are mentioned in Chapter 17, Section 17.8.

### *A-3.1. Input Summary*

**General Information**

| | |
|---|---|
| Process Title: | **BTX from Ethane** |
| Product: | **BTX** |
| Plant Site Location: | **Gulf Coast** |
| Site Factor: | **1.00** |
| Operating Hours per Year: | **7919** |
| Operating Days Per Year: | **330** |
| Operating Factor: | **0.9040** |

**Product Information**

This Process will Yield

| | |
|---|---|
| **114,000** | lb of BTX per hour |
| **2,736,000** | lb of BTX per day |
| **902,770,560** | lb of BTX per year |

Price **$0.41 /lb**

**Chronology**

| Year | Action | Distribution of Permanent Investment | Production Capacity | Depreciation 5 year MACRS | Product Price |
|---|---|---|---|---|---|
| 2015 | Design | | 0.0% | | |
| 2016 | Construction | 100% | 0.0% | | |
| 2017 | Production | 0% | 45.0% | 20.00% | $0.41 |
| 2018 | Production | 0% | 60.0% | 32.00% | $0.42 |
| 2019 | Production | 0% | 75.0% | 19.20% | $0.43 |
| 2020 | Production | | 90.0% | 11.52% | $0.43 |
| 2021 | Production | | 90.0% | 11.52% | $0.44 |
| 2022 | Production | | 90.0% | 5.76% | $0.45 |
| 2023 | Production | | 90.0% | | $0.45 |
| 2024 | Production | | 90.0% | | $0.46 |
| 2025 | Production | | 90.0% | | $0.47 |
| 2026 | Production | | 90.0% | | $0.47 |
| 2027 | Production | | 90.0% | | $0.48 |
| 2028 | Production | | 90.0% | | $0.49 |
| 2029 | Production | | 90.0% | | $0.49 |
| 2030 | Production | | 90.0% | | $0.50 |
| 2031 | Production | | 90.0% | | $0.51 |

**Equipment Costs**

| Equipment Description | | Bare Module Cost |
|---|---|---|
| COL-201 | Process Machinery | $437,618 |
| COL-301 | Process Machinery | $818,588 |
| COL-302 | Process Machinery | $1,380,192 |
| C-201 | Process Machinery | $16,068,648 |
| C-202 | Process Machinery | $16,068,648 |
| PRISM | Fabricated Equipment | $17,000,000 |
| COND-301 | Process Machinery | $57,297 |
| COND-302 | Process Machinery | $174,664 |
| H-201 | Process Machinery | $69,445 |
| H-202 | Process Machinery | $60,689 |
| H-203 | Process Machinery | $70,972 |
| P-201 | Process Machinery | $10,854 |
| P-301 | Process Machinery | $9,747 |
| P-302 | Process Machinery | $12,877 |
| P-303 | Process Machinery | $11,943 |
| P-304 | Process Machinery | $12,990 |
| P-401 | Process Machinery | $43,998 |
| PV-101 | Process Machinery | $1,270,743 |
| RA-301 | Process Machinery | $584,703 |
| RA-302 | Process Machinery | $117,710 |
| RB-301 | Process Machinery | $130,846 |
| RB-302 | Process Machinery | $94,785 |
| ST-204 | Storage | $72,750 |

| | | |
|---|---|---|
| ST-205 | Storage | $72,750 |
| ST-206 | Storage | $72,750 |
| ST-201 | Storage | $418,837 |
| ST-202 | Storage | $418,837 |
| ST-203 | Storage | $418,837 |
| T-101 | Process Machinery | $446,431 |
| T-102 | Process Machinery | $446,431 |
| T-103 | Process Machinery | $446,431 |
| T-104 | Process Machinery | $305,838 |
| T-105 | Process Machinery | $21,360 |
| T-401 | Process Machinery | $194,504 |
| P-101 | Process Machinery | $15,500 |
| P-202 | Process Machinery | $10,818 |
| #REF! | #REF! | #REF! |
| | | |
| Additional Equipment | | $175,810,937 |
| | | |
| **Total** | | ***#REF!*** |

**Raw Materials**

| | Raw Material: | Unit: | Required Ratio: | | Cost of Raw Material: | |
|---|---|---|---|---|---|---|
| 1 | Ethane | lb | 1.6335088 | lb per lb of BTX | $0.067 | per lb |
| 2 | Germanium | kg | 1.001E-05 | kg per lb of BTX | $1,900.00 | per kg |
| 3 | Platinum | kg | 5.22E-06 | kg per lb of BTX | $4,014.20 | per kg |
| 4 | Zeolite | kg | 0.0094668 | kg per lb of BTX | $12.50 | per kg |
| 5 | Alumina | kg | 0.0023667 | kg per lb of BTX | $0.30 | per kg |
| 6 | Chlorine | lb | 0.0118041 | lb per lb of BTX | $0.68 | per lb |
| 7 | Oxygen | lb | 0.0455605 | lb per lb of BTX | $0.09 | per lb |
| 8 | Hydrogen | lb | 0.0074995 | lb per lb of BTX | $0.64 | per lb |
| 9 | Nitrogen | lb | 0.3747448 | lb per lb of | $0.18 | per lb |

BTX

| | | | | | | |
|---|---|---|---|---|---|---|
| | Total Weighted Average: | | | | $0.353 | per lb of BTX |

**Byproducts**

| | Byproduct: | Unit: | Ratio to Product | | Byproduct Selling Price | |
|---|---|---|---|---|---|---|
| 1 | Trimethylbenzene | lb | 0.1026316 | lb per lb of BTX | $0.411 | per lb |
| 2 | Steam (450 psig) | lb | 8.9113158 | lb per lb of BTX | $8.000E-03 | per lb |

| | | | | | | |
|---|---|---|---|---|---|---|
| | Total Weighted Average: | | | | $0.113 | per lb of BTX |

**Utilities**

| | Utility: | Unit: | Required Ratio | | Utility Cost | |
|---|---|---|---|---|---|---|
| 1 | High Pressure Steam | kWh | 0 | kWh per lb of BTX | $0.000E+00 | per kWh |
| 2 | Low Pressure Steam | kWh | 0 | kWh per lb of BTX | $0.000E+00 | per kWh |
| 3 | Process Water | lb | 8.9022692 | lb per lb of BTX | $8.000E-04 | per lb |
| 4 | Cooling Water | lb | 35.422139 | lb per lb of BTX | $1.000E-04 | per lb |
| 5 | Electricity | kWh | 0.3941008 | kWh per lb of BTX | $0.070 | per kWh |
| 6 | Recovered Work | kWh | 0.107126 | kWh per lb of BTX | -$7.000E-02 | per kWh |

| | | | | | | |
|---|---|---|---|---|---|---|
| | Total Weighted | | | | $0.031 | per lb of BTX |

Average:

| #REF! | #REF! | #REF! | | | #REF! |
|---|---|---|---|---|---|

**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** |
| BTX Inventory | ⇨ | **3** | **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: | **8** | **(assuming 5 shifts)** |
| Direct Wages and Benefits: | **$40** | **/operator hour** |

| | | |
|---|---|---|
| Direct Salaries and Benefits: | **15%** | **of Direct Wages and Benefits** |
| Operating Supplies and Services: | **6%** | **of Direct Wages and Benefits** |
| Technical Assistance to Manufacturing: | **$60,000.00** | **per year, for each Operator per Shift** |
| Control Laboratory: | **$65,000.00** | **per year, for each Operator per Shift** |

**Maintenance**

| | | |
|---|---|---|
| Wages and Benefits: | **3.50%** | **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: | **7.10%** | **of Maintenance and Operations Wages and Benefits** |
| Mechanical Department Services: | **2.40%** | **of Maintenance and Operations Wages and Benefits** |
| Employee Relations Department: | **5.90%** | **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: | **2%** | **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** |

## *A-3.2. Cost Summary*

**Variable Cost Summary**

**Variable Costs at 100% Capacity:**

**General Expenses**

| | | | | |
|---|---|---|---|---|
| | Selling / Transfer Expenses: | | $ | 11,198,277 |
| | Direct Research: | | $ | 17,917,244 |
| | Allocated Research: | | $ | 1,866,380 |
| | Administrative Expense: | | $ | 7,465,518 |
| | Management Incentive Compensation: | | $ | 4,665,949 |
| **Total General Expenses** | | | $ | 43,113,367 |
| **Raw Materials** | $0.352842 | per lb of BTX | | $318,535,578 |
| **Byproducts** | $0.113426 | per lb of BTX | | ($102,397,305) |
| **Utilities** | $0.030752 | per lb of BTX | | $27,762,245 |
| **Total Variable Costs** | | | **$** | **287,013,885** |

**Fixed Cost Summary**

**Operations**

| | | | |
|---|---|---|---|
| | Direct Wages and Benefits | $ | 3,328,000 |
| | Direct Salaries and Benefits | $ | 499,200 |
| | Operating Supplies and Services | $ | 199,680 |
| | Technical Assistance to Manufacturing | $ | 2,400,000 |
| | Control Laboratory | $ | 2,600,000 |
| | **Total Operations** | **$** | **9,026,880** |
| **Maintenance** | | | |
| | Wages and Benefits | $ | 10,616,126 |
| | Salaries and Benefits | $ | 2,654,032 |
| | Materials and Services | $ | 10,616,126 |
| | Maintenance Overhead | $ | 530,806 |
| | **Total Maintenance** | **$** | **24,417,091** |
| **Operating Overhead** | | | |
| | General Plant Overhead: | $ | 1,213,912 |
| | Mechanical Department Services: | $ | 410,337 |
| | Employee Relations Department: | $ | 1,008,744 |
| | Business Services: | $ | 1,265,204 |

| | | | |
|---|---|---|---|
| | **Total Operating Overhead** | **$** | **3,898,198** |
| **Property Taxes and Insurance** | | | |
| | Property Taxes and Insurance: | $ | 6,066,358 |
| **Other Annual Expenses** | | | |
| | Rental Fees (Office and Laboratory Space): | $ | - |
| | Licensing Fees: | $ | - |
| | Miscellaneous: | $ | - |
| | **Total Other Annual Expenses** | **$** | **-** |
| **Total Fixed Costs** | | **$** | **43,408,526** |

## Investment Summary

**Total Bare Module Costs:**

| | | |
|---|---|---|
| **Fabricated Equipment** | $ | 192,682,210 |
| **Process Machinery** | $ | 39,395,272 |
| **Spares** | $ | 128,727 |
| **Storage** | | |

| | | | |
|---|---|---|---|
| | $ | 1,474,758 | |
| Other Equipment | $ | - | |
| Catalysts | $ | - | |
| Computers, Software, Etc. | $ | - | |
| **Total Bare Module Costs:** | | | **$ 233,680,967** |
| **Direct Permanent Investment** | | | |
| Cost of Site Preparations: | $ | 11,684,048 | |
| Cost of Service Facilities: | $ | 11,684,048 | |
| Allocated Costs for utility plants and related facilities: | $ | - | |
| **Direct Permanent Investment** | | | **$ 257,049,064** |
| **Total Depreciable Capital** | | | |
| Cost of Contingencies & Contractor Fees | $ | 46,268,832 | |
| **Total Depreciable Capital** | | | **$ 303,317,896** |
| **Total Permanent Investment** | | | |
| Cost of Land: | $ | 6,066,358 | |
| Cost of Royalties: | $ | - | |
| Cost of Plant Start-Up: | $ | 30,331,790 | |
| Total Permanent Investment - Unadjusted | | | |

| | |
|---|---|
| | $ 339,716,043 |
| **Site Factor** | 1.00 |
| **Total Permanent Investment** | **$ 339,716,043** |

## Working Capital

| | 2016 | 2017 | 2018 |
|---|---|---|---|
| Accounts Receivable | $ 13,806,095 | $ 4,602,032 | $ 4,602,032 |
| Cash Reserves | $ 2,632,344 | $ 877,448 | $ 877,448 |
| Accounts Payable | $ (12,808,276) | $ (4,269,425) | $ (4,269,425) |
| BTX Inventory | $ 1,380,610 | $ 460,203 | $ 460,203 |
| Raw Materials | $ 785,430 | $ 261,810 | $ 261,810 |
| **Total** | **$ 5,796,203** | **$ 1,932,068** | **$ 1,932,068** |
| *Present Value at 18%* | *$ 4,912,036* | *$ 1,387,581* | *$ 1,175,916* |

| | |
|---|---|
| **Total Capital Investment** | **$ 347,191,577** |

*A-3.3. Cash Flows*

## Cash Flow Summary

| Year | Percentage of Design Capacity | Product Unit Price | Sales | Capital Costs | Working Capital | Var Costs | Fixed Costs | Depreciation | Depletion Allowance | Taxib |
|---|---|---|---|---|---|---|---|---|---|---|
| 2015 | 0% | | - | - | - | - | - | - | - | |
| 2016 | 0% | | - | (339,716,000) | (5,796,200) | - | - | - | - | |
| 2017 | 45% | $0.41 | 167,974,200 | - | (1,932,100) | (129,156,200) | (43,408,500) | (60,663,600) | - | (65,2 |
| 2018 | 60% | $0.42 | 227,325,000 | - | (1,932,100) | (174,791,500) | (44,059,700) | (97,061,700) | - | (88,5 |
| 2019 | 75% | $0.43 | 288,418,600 | - | (1,932,100) | (221,766,700) | (44,720,500) | (58,237,000) | - | (36,3 |
| 2020 | 90% | $0.43 | 351,293,900 | - | - | (270,111,800) | (45,391,400) | (34,942,200) | - | 848,5 |
| 2021 | 90% | $0.44 | 356,563,300 | - | - | (274,163,500) | (46,072,200) | (34,942,200) | - | 1,385 |
| 2022 | 90% | $0.45 | 361,911,700 | - | - | (278,275,900) | (46,763,300) | (17,471,100) | - | 19,40 |
| 2023 | 90% | $0.45 | 367,340,400 | - | - | (282,450,100) | (47,464,800) | - | - | 37,42 |
| 2024 | 90% | $0.46 | 372,850,500 | - | - | (286,686,800) | (48,176,700) | - | - | 37,98 |
| 2025 | 90% | $0.47 | 378,443,300 | - | - | (290,987,100) | (48,899,400) | - | - | 38,55 |
| 2026 | 90% | $0.47 | 384,119,900 | - | - | (295,351,900) | (49,632,900) | - | - | 39,13 |
| 2027 | 90% | $0.48 | 389,881,700 | - | - | (299,782,200) | (50,377,400) | - | - | 39,72 |
| 2028 | 90% | $0.49 | 395,730,000 | - | - | (304,278,900) | (51,133,000) | - | - | 40,31 |
| 2029 | 90% | $0.49 | 401,665,900 | - | - | (308,843,100) | (51,900,000) | - | - | 40,92 |
| 2030 | 90% | $0.50 | 407,690,900 | - | - | (313,475,800) | (52,678,500) | - | - | 41,53 |
| 2031 | 90% | $0.51 | | - | 11,592,400 | | | - | | |

| | | | | |
|---|---|---|---|---|
| 413,806,300 | (318,177,900) | (53,468,700) | - | 42,15 |

*A-3.4. Profitability Measures*

## Profitability Measures

**The Internal Rate of Return (IRR) for this project is** 2.87%

**The Net Present Value (NPV) of this project in 2015 is** $ (166,765,000)

**ROI Analysis (Third Production Year)**

| | | |
|---|---|---|
| **Annual Sales** | **288,418,629** | |
| **Annual Costs** | **(266,487,209)** | |
| **Depreciation** | **(27,177,283)** | |
| **Income Tax** | **1,940,969** | |
| **Net Earnings** | **(3,304,894)** | |
| **Total Capital Investment** | | **351,308,449** |
| **ROI** | **-0.94%** | |

## Sensitivity Analyses

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

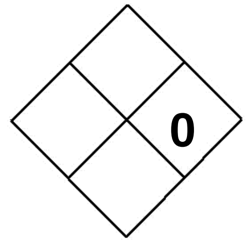
| | Vary Initial Value by +/- |
|---|---|
| x-axis | 15% |
| y-axis | 15% |

**Variable Costs**

| Product Price | $243,961,803 | $252,572,219 | $261,182,636 | $269,793,052 | $278,403,469 | ***$287,013,885*** | $295,624,302 | $304,234,718 | $312,845,135 | $321,455,552 |
|---|---|---|---|---|---|---|---|---|---|---|
| $0.35 | -1.29% | -4.92% | -10.03% | -20.58% | Negative IRR | Negative IRR | Negative IRR | Negative IRR | Negative IRR | Negative IRR |
| $0.36 | 2.40% | -0.36% | -3.71% | -8.18% | -15.73% | Negative IRR | Negative IRR | Negative IRR | Negative IRR | Negative IRR |
| $0.38 | 5.44% | 3.14% | 0.52% | -2.60% | -6.61% | -12.67% | Negative IRR | Negative IRR | Negative IRR | Negative IRR |
| $0.39 | 8.07% | 6.06% | 3.85% | 1.35% | -1.59% | -5.24% | -10.37% | -20.75% | Negative IRR | Negative IRR |
| $0.40 | 10.42% | 8.61% | 6.66% | 4.52% | 2.13% | -0.64% | -4.01% | -8.51% | -16.06% | Negative IRR |
| ***$0.41*** | 12.57% | 10.91% | 9.15% | 7.25% | 5.17% | 2.87% | 0.24% | -2.90% | -6.93% | -13.01% |
| $0.43 | 14.57% | 13.02% | 11.39% | 9.66% | 7.81% | 5.80% | 3.58% | 1.07% | -1.88% | -5.55% |
| $0.44 | 16.44% | 14.99% | 13.46% | 11.86% | 10.17% | 8.36% | 6.40% | 4.26% | 1.85% | -0.93% |
| $0.45 | 18.22% | 16.83% | 15.39% | 13.89% | 12.32% | 10.66% | 8.89% | 6.99% | 4.91% | 2.60% |
| $0.46 | 19.91% | 18.59% | 17.22% | 15.80% | 14.32% | 12.77% | 11.14% | 9.41% | 7.55% | 5.54% |
| $0.48 | 21.54% | 20.26% | 18.95% | 17.60% | 16.19% | 14.73% | 13.21% | 11.61% | 9.91% | 8.10% |

## A-4. MSDS Information

ScienceLab.com
Chemicals & Laboratory Equipment




| | |
|---|---|
| Health | 2 |
| Fire | 3 |
| Reactivity | 0 |
| Personal Protection | H |

# Material Safety Data Sheet

## Benzene MSDS

### Section 1: Chemical Product and Company Identification

**Product Name:** Benzene

**Catalog Codes:** SLB1564, SLB3055, SLB2881

**CAS#:** 71-43-2

**RTECS:** CY1400000

**TSCA:** TSCA 8(b) inventory: Benzene

**CI#:** Not available.

**Synonym:** Benzol; Benzine

**Chemical Name:** Benzene

**Chemical Formula:** C6-H6

**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 |
|---|---|---|
| Benzene | 71-43-2 | 100 |

**Toxicological Data on Ingredients:** Benzene: ORAL (LD50): Acute: 930 mg/kg [Rat]. 4700 mg/kg [Mouse].

DERMAL (LD50): Acute: >9400 mg/kg [Rabbit]. VAPOR (LC50): Acute: 10000 ppm 7 hours [Rat].

## Section 3: Hazards Identification

**Potential Acute Health Effects:**

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

**Potential Chronic Health Effects:**

CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. The substance is toxic to blood, bone marrow, central nervous system (CNS). The substance may be toxic to liver, Urinary System. Repeated or prolonged exposure to the substance can produce target organs damage.

## Section 4: First Aid Measures

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1

**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. WARM water MUST be used. Get medical attention immediately.

**Skin Contact:**

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

**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 if symptoms appear.

**Serious Inhalation:**

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

**Ingestion:**

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

**Serious Ingestion:** Not available.

## Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 497.78°C (928°F)

**Flash Points:** CLOSED CUP: -11.1°C (12°F). (Setaflash)

**Flammable Limits:** LOWER: 1.2% UPPER: 7.8%

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

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

Highly flammable in presence of open flames and sparks, of heat. Slightly flammable to flammable in presence of oxidizing materials. Non-flammable in presence of shocks.

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

Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Explosive in presence of oxidizing materials, of acids.

**Fire Fighting Media and Instructions:**

Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

**Special Remarks on Fire Hazards:**

Extremely flammable liquid and vapor. Vapor may cause flash fire. Reacts on contact with iodine heptafluoride gas. Dioxygenyl tetrafluoroborate is as very powferful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition. Contact with sodium peroxide with benzene causes ignition. Benzene ignites in contact with powdered chromic anhydride. Virgorous or incandescent reaction with hydrogen + Raney nickel (above 210 C) and bromine trifluoride.

**Special Remarks on Explosion Hazards:**

Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction

p.

2

of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid ( or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

## Section 6: Accidental Release Measures

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**

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

## Section 7: Handling and Storage

**Precautions:**

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

**Storage:**

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

## Section 8: Exposure Controls/Personal Protection

**Engineering Controls:**

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

**Personal Protection:**

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

**Personal Protection in Case of a Large Spill:**

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

**Exposure Limits:**

TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States] TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States] TWA: 0.1 STEL: 1 from NIOSH TWA: 1 STEL: 5 (ppm) from OSHA (PEL) [United States] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 3 (ppm) [United Kingdom (UK)] TWA: 1.6 (mg/m3) [United Kingdom

(UK)] TWA: 1 (ppm) [Canada] TWA: 3.2 (mg/m3) [Canada] TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

## Section 9: Physical and Chemical Properties

**Physical state and appearance:** Liquid.

**Odor:**

Aromatic. Gasoline-like, rather pleasant. (Strong.)

**Taste:** Not available.

**Molecular Weight:** 78.11 g/mole

**Color:** Clear Colorless. Colorless to light yellow. **pH (1% soln/water):** Not available.

**Boiling Point:** 80.1 (176.2°F)

**Melting Point:** 5.5°C (41.9°F)

**Critical Temperature:** 288.9°C (552°F)

**Specific Gravity:** 0.8787 @ 15 C (Water = 1)

**Vapor Pressure:** 10 kPa (@ 20°C)

**Vapor Density:** 2.8 (Air = 1)

**Volatility:** Not available.

**Odor Threshold:** 4.68 ppm

**Water/Oil Dist. Coeff.:** The product is more soluble in oil; log(oil/water) = 2.1

**Ionicity (in Water):** Not available.

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

**Solubility:**

Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water.

## Section 10: Stability and Reactivity Data

**Stability:** The product is stable.

**Instability Temperature:** Not available.

**Conditions of Instability:** Heat, ignition sources, incompatibles.

**Incompatibility with various substances:** Highly reactive with oxidizing agents, acids.

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

**Special Remarks on Reactivity:**

Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid ( or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

**Special Remarks on Corrosivity:** Not available.

**Polymerization:** Will not occur.

## 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): 930 mg/kg [Rat]. Acute dermal toxicity (LD50): >9400 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 10000 7 hours [Rat].

**Chronic Effects on Humans:**

CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. Causes damage to the following organs: blood, bone marrow, central nervous system (CNS). May cause damage to the following organs: liver, Urinary System.

**Other Toxic Effects on Humans:**

Very hazardous in case of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion.

**Special Remarks on Toxicity to Animals:** Not available.

**Special Remarks on Chronic Effects on Humans:**

May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic, leukemia)) Human: passes the placental barrier, detected in maternal milk.

**Special Remarks on other Toxic Effects on Humans:**

Acute Potential Health Effects: Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism,and urinary system. Eyes: Causes eye irritation. Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/Central and Peripheral nervous systems (somnolence, muscle weakness, general anesthetic, and other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system. Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood.

## Section 12: Ecological Information

**Ecotoxicity:** Not available.

**BOD5 and COD:** Not available.

**Products of Biodegradation:**

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

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

**Special Remarks on the Products of Biodegradation:** Not available.

## Section 13: Disposal Considerations

**Waste Disposal:**

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

## Section 14: Transport Information

**DOT Classification:** CLASS 3: Flammable liquid.

**Identification:** : Benzene UNNA: 1114 PG: II

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

## Section 15: Other Regulatory Information

**Federal and State Regulations:**

California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene California prop. 65 (no significant risk level): Benzene: 0.007 mg/day (value) California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer which would require a warning under the statute: Benzene Connecticut carcinogen reporting list.: Benzene Connecticut hazardous material survey.: Benzene Illinois toxic substances disclosure to employee act: Benzene Illinois chemical safety act: Benzene New York release reporting list: Benzene Rhode Island RTK hazardous substances: Benzene Pennsylvania RTK: Benzene Minnesota: Benzene Michigan critical material: Benzene Massachusetts RTK: Benzene Massachusetts spill list: Benzene New Jersey: Benzene New Jersey spill list: Benzene Louisiana spill reporting: Benzene California Director's list of Hazardous Substances: Benzene TSCA 8(b) inventory: Benzene SARA 313 toxic chemical notification and release reporting: Benzene CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.536 kg)

**Other Regulations:**

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

**Other Classifications:**

**WHMIS (Canada):**

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

**DSCL (EEC):**

R11- Highly flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes. R45- May cause cancer. R62- Possible risk of impaired fertility. S2- Keep out of the reach of children. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S39- Wear eye/face protection. S46- If swallowed, seek medical advice immediately and show this container or label. S53- Avoid exposure - obtain special instructions before use.

**HMIS (U.S.A.):**

**Health Hazard:** 2

**Fire Hazard:** 3

**Reactivity:** 0

**Personal Protection:** h

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

**Health:** 2

**Flammability:** 3

**Reactivity:** 0

**Specific hazard:**

**Protective Equipment:**

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

## Section 16: Other Information

**References:** Not available.

**Other Special Considerations:** Not available.

**Created:** 10/10/2005 08:35 PM

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

# MATERIAL SAFETY DATA SHEET

**SECTION 1. PRODUCT**

**IDENTIFICATION PRODUCT NAME:** **Carbon Dioxide**

**CHEMICAL NAME:** Carbon Dioxide **FORMULA:** $CO_2$

**SYNONYMS:** Carbonic Anhydride, Carbonic Acid Gas, Carbon Anhydride

**MANUFACTURER:** **Air Products and Chemicals, Inc.**

7201 Hamilton Boulevard

Allentown, PA 18195-1501

**PRODUCT INFORMATION:** 1 - 800 - 752 - 1597

**MSDS NUMBER:** 1005 **REVISION:** 5

**REVISION DATE:** March 1993 **REVIEW**

**DATE:** March

1994

**SECTION 2. COMPOSITION / INFORMATION ON**

**INGREDIENTS CONCENTRATION:** Carbon dioxide is sold as pure product

> 99%.

**CAS NUMBER:** 124-38-9

**EXPOSURE LIMITS:**

**OSHA:** PEL-TWA = 5000 ppm **ACGIH:** TLV-TWA = 5000 ppm
**NIOSH:** None established

**SECTION 3. HAZARDS IDENTIFICATION**

**EMERGENCY OVERVIEW**

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

**EMERGENCY TELEPHONE NUMBERS**

**800 - 523 - 9374** **Continental U.S., Canada, or Puerto Rico**

**610 - 481 - 7711 other locations**

**POTENTIAL HEALTH EFFECTS:**

**INHALATION:** Carbon dioxide is an asphyxiant. Concentrations of 10% or more can produce unconsciousness or death.

**EYE CONTACT:** Contact with liquid or cold vapor can cause freezing of tissue.

**SKIN CONTACT:** Contact with liquid or cold vapor can cause frostbite.

**EXPOSURE INFORMATION:**

**ROUTE OF ENTRY:**

Inhalation

**TARGET ORGANS:** Central nervous system

**EFFECT:** Asphyxiation (suffocation). Overexposure may cause damage to retinal ganglion cells and central nervous system.

**SYMPTOMS:** Headache, sweating, rapid breathing, increased heartbeat, shortness of breath, dizziness, mental depression, visual disturbances, and shaking.

**CHRONIC EFFECTS:** None established.

**MEDICAL CONDITIONS AGGRAVATED BY OVEREXPOSURE:** None

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

## SECTION 4. FIRST AID

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

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

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

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

## SECTION 5. FIRE AND EXPLOSION

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

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

**HAZARDOUS COMBUSTION PRODUCTS:** None known.

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

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

## SECTION 6. ACCIDENTAL RELEASE MEASURES

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

## SECTION 7. HANDLING AND STORAGE

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

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

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

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

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

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

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

## SECTION 8. PERSONAL PROTECTION / EXPOSURE CONTROL

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

**RESPIRATORY PROTECTION:**

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

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

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

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

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

**MOLECULAR WEIGHT:** 44.01

**GAS DENSITY (at 70 °F (21.1 °C) and 1 atm):** 0.1144 lb/ft$^3$ (1.832 kg/m$^3$)

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

**SPECIFIC GRAVITY (Air =1):** 1.522

**SPECIFIC VOLUME (at 70 F (21.1 C) and 1 atm):** 8.74 $ft^3/lb$ (0.5457 $m^3/kg$)

**BOILING POINT:** -109.3 F (-78.5 C)

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

**SOLUBILITY IN WATER (Vol./Vol. at 68 F (20 C)):** 0.90

## SECTION 10. STABILITY AND REACTIVITY

**STABILITY:**
Stable

**CONDITIONS TO AVOID:** None

**INCOMPATIBILITY (Materials to Avoid):**
None **REACTIVITY:**

**HAZARDOUS DECOMPOSITION PRODUCTS:** None

**HAZARDOUS POLYMERIZATION:** Will not occur

## SECTION 11. TOXICOLOGICAL INFORMATION

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

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

## SECTION 12. ECOLOGICAL INFORMATION

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

## SECTION 13.

## DISPOSAL

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

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

## SECTION 14. TRANSPORT INFORMATION

**DOT SHIPPING NAME:** Carbon dioxide **HAZARD CLASS:** 2.2 (Nonflammable Gas) **IDENTIFICATION NUMBER:** UN1013

**PRODUCT RQ:** None

**SHIPPING LABEL(s):** Nonflammable gas

**PLACARD (when required):** Nonflammable gas

~~**SPECIAL SHIPPING INFORMATION:** Cylinders should be transported in a secure upright~~ position in a well ventilated truck. Never transport in passenger compartment of a vehicle.

**SECTION 15. REGULATORY**

**INFORMATION U.S. FEDERAL REGULATIONS:**

**ENVIRONMENTAL PROTECTION AGENCY (EPA):**

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

CERCLA Reportable Quantity: None.

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

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

Extremely Hazardous Substances: None

Threshold Planning Quantity (TPQ): None

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

IMMEDIATE HEALTH: Yes

PRESSURE: Yes DELAYED HEALTH: No

REACTIVITY: No FLAMMABLE: No

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

Carbon dioxide does not require reporting under Section 313

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

Carbon dioxide is not listed as a regulated substance.

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

**OSHA - OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION:**

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

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

**STATE REGULATIONS:**

CALIFORNIA:

Proposition 65: This product does NOT contain any listed substances which the State of California requires warning under this statute. SCAQMD Rule: VOC = Not applicable

## SECTION 16. OTHER INFORMATION

**HAZARD RATINGS:**

**NFPA RATINGS:**

**HMIS RATINGS:**

| NFPA | | HMIS | |
|---|---|---|---|
| HEALTH: | 1 | HEALTH: | 0 |
| FLAMMABILITY: | 0 | FLAMMABILITY: | 0 |
| REACTIVITY: | 0 | REACTIVITY: | 0 |
| SPECIAL: | SA* | | |

*Compressed Gas Association recommendation to designate simple asphyxiant.

Revision information: New format with additional sections added. Reformatted September 1998.

# Safety Data Sheet
# CHLORINE

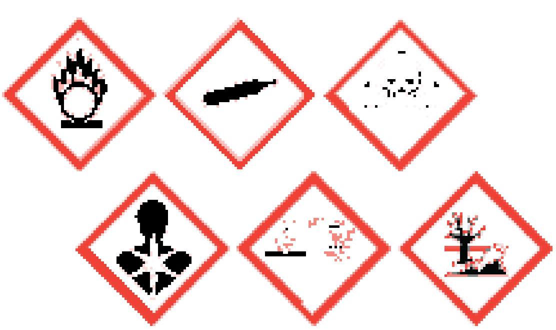
MVC-MSDS-C-001P Issue Date : 04/15/15 Rev. Code : 03-A Page 1 of 5

## I. PRODUCT AND COMPANY IDENTIFICATION

| | |
|---|---|
| Product Name | Liquid Chlorine |
| Recommended use of the chemical and restrictions on use | Used in water treatment and disinfection; as bleaching agent, particularly for paper and textiles; in the manufacture of bleaching powder and chemicals such as PVC, chlorinated hydrocarbons, ethylene glycol, glycerine and tetraethyl lead. |
| | Chlorine is 2.5 times heavier than air. It is not an explosive or flammable gas, but reacts violently with oils, solvents, grease, ammonia, acetone, etc. |
| Manufacturer | Mabuhay Vinyl Corporation<br>3rd Floor Philamlife, 126 L.P. Leviste St. Salcedo Village, Makati City<br>For Assistance Call : (02) 817-8971 to 76 loc 214; Direct line (02) 817-1830 |
| Iligan Plant | Assumption Heights, Iligan City<br>Tel: (063) 221-9466, 221-1190 |
| Mabuhay Premium Bleach Plant | LTAI, Brgy. Biñan, Biñan, Laguna<br>Tel: (049) 541-1923 |
| Batangas Depot | BBTI Compound, Bauan, Batangas<br>Tel: (043) 980-5869 |
| Cebu Depot | Ceniza St., Ouano, Mandaue City<br>Tel: (032) 344-5259, 345-0639 |
| Davao Depot | Bunawan, Davao City<br>Tel: (082) 236-0015 |

## II. HAZARDS IDENTIFICATION

Symbols



Precautionary statements:

Prevention

P220: Keep/Store away from clothing/combustible materials.
P244: Keep reduction valves free from grease and oil.
P261: Avoid breathing dust/fume/gas/mist/vapours/spray.
P264: Wash thoroughly after handling.
P280: Wear protective gloves/protective clothing/eye protection/face protection.
P284: Wear respiratory protection.
P271: Use only outdoors or in a well- ventilated area
P273: Avoid release to the environment.

Response:

P370+P376: In case of fire: Stop leak if safe to do so
P304+P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P301 + P330 + P331: IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
P305+P351+P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313: If eye irritation persists: Get medical advice/ attention.
P303 + P361 + P353: IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower
P363: Wash contaminated clothing before reuse
P310: Immediately call a POISON CENTER or doctor/physician.
P312: Call a POISON CENTER or doctor/physician if you feel unwell.
P320: Specific treatment is urgent (see MSDS).
P391 Collect spillage.

Storage:

P403: Store in a well ventilated place.
P410: Protect from sunlight
P233: Keep container tightly closed.
P405: Store locked up.

Disposal:

P501: Dispose of contents/container in accordance with applicable local, regional, national, and/or international regulations

## III. COMPOSITION / INFORMATION ON INGREDIENTS

# Safety Data Sheet
# CHLORINE



## IV. FIRST AID MEASURES

Description of first-aid measures: In all instances, seek immediate medical attention. Show this safety data sheet to the physician in attendance.

In case of frostbite place the frostbitten part in warm water. Do not use hot water! If warm water is not available wrap the affected parts gently in blankets. Encourage victim to gently exercise the affected part while being warmed. Seek immediate medical attention.

Inhalation: Remove to fresh air. Give artificial respiration if not breathing, preferably mouth-to-mouth . If breathing is difficult, administer oxygen. Keep the affected person warm at rest. In mild cases, give milk to relieve throat irritation.

Ingestion: Not a likely route of exposure.

Skin contact: Wash with plenty of soap and water while removing contaminated clothing and shoes. Get medical attention. Wash clothing before reuse. Destroy contaminated shoes. Do not apply greases unless ordered by a physician.

Eye contact: Immediately flush eyes with a directed stream of water for at least 15 minutes, forcibly holding eyelids apart to ensure complete irrigation of all eye and lid tissues. Washing eyes within several seconds is essential to achieve maximum effectiveness. Do not attempt chemical neutralization of any kind.

Most important symptoms/effects, both acute and delayed

Toxic and irritating, with Inhalation as the major potential route of exposure. May cause severe irritation of mucous membranes of the nose, throat and respiratory tract followed by severe coughing, burning, chest pain, vomiting, headache, anxiety and feeling of suffocation. Severe breathing difficulties may occur which may be delayed in onset. Severe exposure may lead to chemical pneumonitis and pulmonary edema and may be fatal. Repeated or prolonged exposure may result in reduced pulmonary capacity and dental erosion.

Skin contact with liquid chlorine may cause serious burns, blistering and tissue destruction. Chlorine vapors can cause irritation, burning and blisters. Contact with rapidly expanding gas poses a frostbite hazard.

Indication of any immediate medical attention and special treatment needed: No known antidote. Treatment for inhalation is symptomatic and supportive. Keep patient at rest until respiratory symptoms subside. Sedation for apprehension or restlessness may be considered as well as diuretics and antibiotics to alleviate edema and protect against secondary infection. Administer oxygen under exhalation pressure not exceeding 4 cm water for 15 minutes each hour until symptoms subside (except in presence of impending or existing cardiovascular failure). Steroid therapy, if given early, has been reported effective in preventing pulmonary edema. It is recommended that anyone exposed to chlorine gas by inhalation obtain a chest x-ray to check for pulmonary edema.

First Aid Facilities: Eye wash station, safety shower and normal washroom facilities.

## V. FIRE FIGHTING MEASURES

Extinguishing media

Suitable extinguishing media: Water spray, fog or foam. For large fires, flood with fine water spray. Use water to keep fire - exposed containers cool and continue until well after fire is out.

Unsuitable extinguishing media: Do not use carbon dioxide or halogenated extinguishing agents.

Special hazards arising from the substance or mixture: Although non-flammable, chlorine is a strong oxidizer and may react to cause fire and/or explosion upon contact with turpentine, ether, ammonia, hydrocarbons, certain metal hydrides, carbides, nitrides, oxides, sulfides, phosphides, easily oxidized materials, organic materials or other flammables. It forms corrosive Hydrogen Chloride on contact with water. Chlorine gas is heavier than air and will collect in low-lying areas.

Special protective actions for firefighters: Self-contained breathing equipment, eye protection and full protective clothing is required. Move container from fire area if it can be done without risk. Stay away from the ends of tanks. Keep unnecessary people away, isolate hazard area and deny entry. Cool containers with water spray until well after the fire is out. Apply water from a protected location or from a safe distance. Avoid inhalation of material or combustion by-products. Stay upwind and keep out of low areas. Evacuation radius: 800 meters (1/2 mile). Do not allow contaminated extinguishing water to enter the soil, groundwater or surface waters.

## VI. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures: Evacuate all unprotected personnel. Put on protective equipment (see Section 8). Avoid direct contact with skin, eyes and clothing. Ensure adequate ventilation/exhaust extraction. Avoid low-lying areas. Work upwind if possible.

Environmental precautions: Avoid entry of product into drains, sewers, surface/ground water system or soil. Drains for storage or use areas should have retention basins for pH adjustments and dilution of spills before discharge or disposal of material.

Methods and material for containment and cleaning up: When possible, move leaking or damaged cylinders outdoors or to an isolated location. If source of leak is a cylinder and the leak cannot be stopped in place, remove the leaking cylinder to a safe place in the open air and repair the leak or allow the cylinder to empty through a reducing agent such as caustic soda, soda ash, or hydrated lime solutions. Turn leaking cylinder with the leak up to prevent escape of gas in liquid state. Chlorine vapors are heavier than air, and pockets of chlorine are likely to be trapped in low lying areas. Use water fog to dampen a chlorine cloud and reduce vapours. Do not spray water directly on the leak or chlorine container. Liquid or solid residues must be disposed of in accordance with all applicable regulations.

## VII. HANDLING AND STORAGE

Precautions for safe handling: Use protective equipment (see Section 8). Provide adequate ventilation. Avoid inhalation of vapors and skin and eye contact. Change contaminated or soaked clothing immediately. Wash hands after handling.

Provide special training to workers handling chlorine. Regularly test and inspect piping and containment used for chlorine service. Liquid levels should be less than 85% of tank or cylinder capacity.

Do not drag, slide or roll cylinders. Use a suitable hand truck for cylinders movement. Protect cylinders and containers from physical damage. Keep containers tightly closed when not in use. Chlorine emergency equipment should be available near the point of use.

Keep away from foodstuffs, drinks and tobacco.

Keep away from incompatible products.

Conditions for safe storage, including any incompatibilities

Store chlorine containers and cylinders below 45°C in cool, dry, well ventilated areas of non-combustible construction away from sunlight, precipitation, heavily trafficked areas and emergency exit. Cylinders should be stored upright and firmly secured to prevent falling or being knocked over. Full and empty cylinders should be segregated. Full cylinders should not be stored for more than six months. Liquid levels should be less than 85 % of container or cylinder capacity.

Non suitable packaging material: Acetal , aluminum, brass, Bronze, carbon steel, cast iron, chrome, CPVC, epoxy, LDPE, natural rubber, neoprene, nitrile, nylon, polyether-ether ketone(PEEK) , polypropylene, polyurethane, PPS, PVC, silicone, titanium

Keep away from heat, sparks, open flames and incompatible substances(see Section X).

## VIII. EXPOSURE CONTROLS AND PROTECTION

Control parameters

| | |
|---|---|
| ACGIH | 0.5 ppm TWA<br>1 ppm STEL |
| Europe | 0.5 ppm STEL; 1.5 mg/m3 STEL |
| OSHA (Final) | 1 ppm Ceiling; 3 mg/m3 Ceiling |
| OSHA (Vacated) | 0.5 ppm TWA; 1.5 mg/m3 TWA<br>1 ppm STEL; 3 mg/m3 STEL |
| NIOSH | 0.5 ppm Ceiling (15 min); 1.45 mg/m3 Ceiling (15 min) |
| Philippines | 3 mg/m3 (TWA) OEL 1 ppm (TWA) OEL |

Appropriate engineering controls: A system of local and / or general exhaust is recommended to keep employee exposure as low as possible. Use enclosed, isolated processing and handling whenever possible.

Personal protective equipment

Maintain eye wash fountain and quick-drench facilities in work area. Final choice of appropriate protection will vary according to methods of handling, engineering controls and risk assessments undertaken.

Respiratory protection NIOSH-approved full- or half - face piece (with goggles) respiratory protective equipment

Up to 5 ppm:

Any chemical cartridge respirator with cartridge(s) providing protection against the compound of concern

Any supplied-air respirator

Up to 10 ppm:

Any supplied-air respirator operated in a continuous-flow mode

Any powered, air-purifying respirator with cartridge(s) providing protection against the compound of concern

Any chemical cartridge respirator with a full facepiece and cartridge(s) providing protection against the compound of concern

Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted canister providing protection against the compound of concern

Any self-contained breathing apparatus with a full facepiece

Any supplied-air respirator with a full facepiece

Emergency or planned entry into unknown concentrations or IDLH conditions:

Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode

Any supplied-air respirator that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained positive-pressure breathing apparatus

Escape:

Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted canister providing protection against the compound of concern

Any appropriate escape-type, self-contained breathing apparatus

Hand protection: PVC, rubber or neoprene gloves

Eye / face protection: splash-proof safety goggles with side shields or face shield

Skin protection: Appropriate impermeable protective clothing(made of Viton, butyl rubber, Teflon, chlorinated polyethylene material ) to protect against possible skin contact. When responding to accidental release of unknown concentrations, wear one-piece, total encapsulating suit of Butyl coated nylon or equivalent.

# Safety Data Sheet
# CHLORINE



## IX. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|---|---|
| Appearance | Greenish-yellow to amber gas |
| Odor | Irritating, pungent odor |
| Odor threshold | 0.2ppm |
| pH | Not applicable |
| Freezing point | -101°C |
| Boiling point /range | -34°C |
| Flash point | Not applicable |
| Evaporation rate | Not applicable |
| Flammability | Non flammable |
| Flammability/explosive limits | Not applicable |
| Vapor pressure | 5168 mm Hg at 21°C |
| Vapor density | 2.49 (air = 1.0) |
| Relative density(water = 1) | 1.41 at 20°C(liquid) |
| Solubility(in water) | 14.6gpl at 0°C; 6.9gpl at 20°C |
| Partition coefficient: n-octanol/water | Not available |
| Auto-ignition temperature | Not applicable |
| Decomposition temperature | Not available |
| Viscosity | 14 Pa.s at 20°C |

## X. STABILITY AND REACTIVITY

Reactivity: May react violently with combustible materials. Reacts with water to form corrosive acids. May react violently with alkalis. With water causes rapid corrosion of some metals. May react violently with reducing agents. Violently oxidises organic material.

Stability: Stable under recommended storage conditions.

Possibility of hazardous reactions or polymerization: Will not polymerize. Reacts violently with a variety of substances over a broad range of conditions including reducing agents and combustible materials.

Conditions to avoid: Heat, sparks, sunlight, moisture and incompatible substances.

## XI. TOXICOLOGICAL INFORMATION

Routes of exposure: inhalation, ingestion, skin and eye contact

Symptoms related to the physical, chemical and toxicological characteristics: causes severe irritation of the eyes and respiratory tract with eye injury, restlessness, shortness of breath, cough, choking sensation, sneezing, running nose, chest pain, dizziness, headache, nausea, cyanosis (lack of oxygen in the blood) and respiratory failure. Following respiratory tract injury, onset of severe breathing difficulties, including bronchitis, lung edema (accumulation of fluid in the lungs) and pneumonia, may be delayed and life threatening.

Delayed and immediate effects and also chronic effects from short and long term exposure: High concentrations of chlorine over a short period of time may aggravate pre-existing heart conditions, and cause congestive heart failure. At high concentrations, chlorine gas irritates the skin and can produce sensations of burning and pricking of the skin, with inflammation and blister formation. Exposure to concentrations as low as 5-10 ppm is reported to cause severe irritation of the eyes, nose and respiratory tract which is intolerable after a few minutes.

Numerical measures of toxicity The hazards via inhalation at different concentrations is reported to be as follows:

| | |
|---|---|
| 0.2-0.5 ppm | No toxic, long term effect |
| 1-3 ppm | Definite odor: irritation of eyes and nose |
| 5-8 ppm | Throat, eye, and mucous membrane irritation |
| 30 ppm | Intense coughing fits |
| 34-51 ppm | Lethal in 1 to 1.5 hours exposure |
| 40-60 ppm | Exposure for 30-60 minutes without effective respiration may cause bronchitis, pulmonary edema or bronchopneumonia |
| 100 ppm | May be lethal after 50 minutes of exposure (estimated) |
| 430 ppm | Lowest concentration known to cause lethality after 30 minutes of exposure |
| 1000 ppm | May be fatal with a few deep breaths |

Incompatible materials: Hydrocarbons, combustible materials, bases, acids, metals, metal salts, carbides, oxides, phosphides, nitrides, sulfides, reducing agents, oxidizing materials, halogens, halo carbons, amines, ammonia, arsenic, calcium, iodine, ethers, fluorine

Hazardous decomposition products: Does not decompose but reacts violently to form hydrochloric acid and other potentially toxic and/ or corrosive substances.

## XII. ECOLOGICAL INFORMATION

Ecotoxicity

FISH TOXICITY: 390 ug/L 96 hour(s) LC50 (Mortality) Orangethroat darter (Etheostoma spectabile)

INVERTEBRATE TOXICITY: 637.5 ug/L 1 hour(s) LC50 (Mortality) Pacific oyster (Crassostrea gigas)

ALGAL TOXICITY: 50-1000 ug/L 23 hour(s) (Population) Algae,phytoplankton,algal mat (Algae)

PHYTOTOXICITY: 20 ug/L 96 day(s) (Growth) Water-milfoil (Myriophyllum spicatum)

# Safety Data Sheet
# CHLORINE



Persistence and degradability:

Biodegradation (In water): Half-life: 1.3 to 5 hours.

Photodegradation (In air) : Half-life: 10 minutes, lifetime: 14 minutes.

Bioaccumulative potential : An accumulation in aquatic organisms is not to be expected

Mobility

In water, chlorine is transformed to free available chlorine (gaseous chlorine), hypochlorous acid and hypochlorite ions, whose relative amounts depend on the pH and other physicochemical properties of the water. At environmental pH, only hypochlorous acid and hypochlorite will be present.

In the atmosphere, $Cl_2$ will degrade during daylight, with half-lives ranging from minutes to several hours, depending on latitude, season, and time of day.

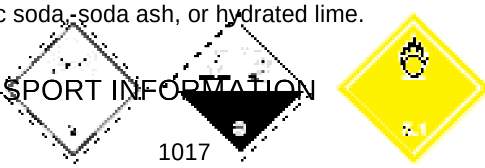
In soil, the high water solubility of chlorine can lead to a high mobility in soil, although chlorine as vapour or as aqueous solution is normally irreversibly bound to soil organics within the first few millimeters or centimeters of the soil surface.

## XIII. DISPOSAL CONSIDERATIONS

Dispose of in accordance with all Government and Local regulations. Container is returnable and must be properly identified with return tag and returned as promptly as possible to supplier, in accordance with all applicable DOT regulations. All valves must be closed tight and closures or caps secured. It is illegal to ship a leaking Chlorine container.

Chlorine gas will disperse to the atmosphere leaving no residue. When possible, move leaking container to an isolated area. Position to release gas, not liquid. Absorb in alkaline solution of caustic soda, soda ash, or hydrated lime.

## XIV. TRANSPORT INFORMATION



| | |
|---|---|
| UN Number | 1017 |
| UN Proper Shipping Name | CHLORINE |
| Transport hazard class | 2.3(Toxic Gas, Corrosive, Oxidizing) |
| Packing group | Not applicable |

Label

Environmental Hazards

| | | |
|---|---|---|
| Marine Pollutant : | Yes | IMDG |
| Environmentally Hazardous : | Yes | ADR/RID |
| | No | IATA |

Special precautions

Transport in open ventilated vehicle, cylinders upright and secured, drum placed lengthwise in the truck tray, with the valve end facing away from the vehicle. Do not transport in confined spaces like refrigerated compartments of vehicles, truck cabs or in passenger compartments. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency.

## XV. REGULATORY INFORMATION

U.S. Regulations:

This material contains one or more of the following chemicals required to be identified under SARA Section 302/304 (40 CFR 355 Appendix A), SARA Section 313 (40 CFR 372.65), CERCLA (40 CFR 302.4), TSCA 12(b), and/or require an OSHA process safety plan.

CHLORINE (7782-50-5)
SARA 302: 100 lb TPQ
SARA 304: 10 lb EPCRA RQ
SARA 313: 1.0 % de minimis concentration CERCLA: 10 lb final RQ; 4.54 kg final RQ OSHA: 1500 lb TQ

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

Acute: Yes Chronic: No Fire: No Reactive: No Sudden release: No

National Inventories

Australian Chemical Inventory(AICS) : Listed Canadian Chemical Inventory(DSL) : Listed China Chemical Inventory(IECS ): Listed European Union Inventory(EINECS) : 231-959-5 Japan Chemical Inventory(ENCS ): Not listed Korean Chemical Inventory(KECL) : KE-05486 New Zealand Chemical Inventory(NZIOC) : Listed

Philippines - Priority Chemical List(PICCS) : Listed U.S. Inventory (TSCA) : Listed

## XVI. OTHER INFORMATION

The information herein is presented in good faith and believed to be correct as of the date of issue. However, no warranty, expressed or implied, is made by Mabuhay Vinyl Corporation regarding the product's merchantability, fitness for a particular purpose, performance, safety or stability. This information is not intended to be all-inclusive as to the manner and conditions of use, handling, storage, disposal and other factors that may involve other or additional legal, environmental, safety or performance considerations, and Mabuhay Vinyl Corporation assumes no liability whatsoever for the use of or reliance upon this information. No suggestions for use are intended as, and nothing herein shall be construed as, a recommendation to infringe any existing patents or to violate any existing laws or regulations.

THE LINDE GROUP

Linde

# Safety data sheet
# Ethane

| | | | | |
|---|---|---|---|---|
| Creation date : | 28.01.2005 | Version : 2.0 | DE / E | SDS No. : 051a |
| Revision date : | 04.01.2011 | | | page 1 / 3 |

## 1 IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY

**Product name**
Ethane
EC No (from EINECS): 200-814-8
CAS No: 74-84-0
Index-Nr. 601-002-00-X
**Chemical formula** C2H6
**REACH Registration number**:
Not available.
**Known uses**
Not known.
**Company identification**
Linde AG, Linde Gas Division, Seitnerstraße 70, D-82049 Pullach
**E-Mail Address** Info@de.linde-gas.com
**Emergency phone numbers (24h):** 089-7446-0

## 2 HAZARDS IDENTIFICATION

**Classification of the substance or mixture**

**Classification acc. to Regulation (EC) No 1272/2008/EC (CLP/GHS)**
Press. Gas (Liquefied gas) - Contains gas under pressure; may explode if heated.
Flam. Gas 1 - Extremely flammable gas.

**Classification acc. to Directive 67/548/EEC & 1999/45/EC**
F+; R12
Extremely flammable.
**Risk advice to man and the environment**
Liquefied gas.
Contact with liquid may cause cold burns/frost bite.
**Label Elements**

**- Labelling Pictograms**

**- Signal word**
Danger

**- Hazard Statements**

| | |
|---|---|
| H280 | Contains gas under pressure; may explode if heated. |
| H220 | Extremely flammable gas. |

**- Precautionary Statements**

**Precautionary Statement Prevention**

| | |
|---|---|
| P210 | Keep away from heat/sparks/open flames/hot surfaces. - No smoking. |

**Precautionary Statement Reaction**

| | |
|---|---|
| P377 | Leaking gas fire: Do not extinguish, unless leakcan be stopped safely. |
| P381 | Eliminate all ignition sources if safe to do so. |

**Precautionary Statement Storage**

| | |
|---|---|
| P403 | Store in a well-ventilated place. |

**Precautionary Statement Disposal**
None.

## 3 COMPOSITION/INFORMATION ON INGREDIENTS

**Substance/Preparation:** Substance.
**Components/Impurities**
Ethane
**CAS No:** 74-84-0
**Index-Nr.**: 601-002-00-X
**EC No (from EINECS):** 200-814-8
**REACH Registration number**:
Not available.
Contains no other components or impurities which will influence the classification of the product.

## 4 FIRST AID MEASURES

**Inhalation**
In high concentrations may cause asphyxiation. Symptoms may include loss of mobility/consciousness. Victim may not be aware of asphyxiation. In low concentrations may cause narcotic effects. Symptoms may include dizziness, headache, nausea and loss of co-ordination. Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
**Skin/eye contact**
For liquid spillage - flush with water for at least 15 minutes Obtain medical assistance.
**Ingestion**
Ingestion is not considered a potential route of exposure.

## 5 FIRE FIGHTING MEASURES

**Specific hazards**
Exposure to fire may cause containers to rupture/explode.
**Hazardous combustion products**
Incomplete combustion may form carbon monoxide.
**Suitable extinguishing media**
All known extinguishants can be used.
**Specific methods**
If possible, stop flow of product. Move container away or cool with water from a protected position. Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.
**Special protective equipment for fire fighters**
In confined space use self-contained breathing apparatus.

## 6 ACCIDENTAL RELEASE MEASURES

**Personal precautions**
Wear self-contained breathing apparatus when entering area unless atmosphere is proved to be safe. Evacuate area. Ensure adequate air ventilation. Eliminate ignition sources.
**Environmental precautions**
Try to stop release. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.
**Clean up methods**
Ventilate area. Keep area evacuated and free from ignition sources until any spilled liquid has evaporated. (Ground free from frost).

## 7 HANDLING AND STORAGE

**Handling**
Ensure equipment is adequately earthed. Suck back of water into the container must be prevented. Purge air from system before

THE LINDE GROUP

Linde

# Safety data sheet
# Ethane

| | | | | |
|---|---|---|---|---|
| Creation date : | 28.01.2005 | Version : 2.0 | DE / E | SDS No. : 051a |
| Revision date : | 04.01.2011 | | | page 2 / 3 |

introducing gas. Do not allow backfeed into the container. Use only properly specified equipment which is suitable for this product, its supply pressure and temperature. Contact your gas supplier if in doubt. Keep away from ignition sources (including static discharges). Refer to supplier's handling instructions.

**Storage**

Secure cylinders to prevent them falling. Segregate from oxidant gases and other oxidants in store. Keep container below 50°C in a well ventilated place. Observe "Technische Regeln Druckgase (TRG) 280 Ziffer 5"

## 8 EXPOSURE CONTROLS/PERSONAL PROTECTION

**Personal protection**

Ensure adequate ventilation. Do not smoke while handling product. Carry working gloves and protection shoes while handling gas cylinders.

## 9 PHYSICAL AND CHEMICAL PROPERTIES

**General information**

**Appearance/Colour:** Colourless gas.

**Odour:** None. Stenchant often added

**Important information on environment, health and safety**

**Molecular weight:** 30 g/mol

**Melting point:** -183 °C

**Boiling point:** -88,6 °C

**Critical temperature:** 32 °C

**Autoignition temperature:** 515 °C

**Flammability range:** 2,7 %(V) - 16 %(V)

**Relative density, gas:** 1

**Relative density, liquid:** 0,54

**Vapour Pressure 20 °C:** 37,8 bar

**Solubility mg/l water:** 61 mg/l

**Other data**

Gas/vapour heavier than air. May accumulate in confined spaces, particularly at or below ground level.

## 10 STABILITY AND REACTIVITY

**Stability and reactivity**

Can form explosive mixture with air. May react violently with oxidants.

## 11 TOXICOLOGICAL INFORMATION

**Acute toxicity**

No known toxicological effects from this product.

## 12 ECOLOGICAL INFORMATION

**General**

No known ecological damage caused by this product.

## 13 DISPOSAL CONSIDERATIONS

**General**

Do not discharge into areas where there is a risk of forming an explosive mixture with air. Waste gas should be flared through a suitable burner with flash back arrestor. Do not discharge into any place where its accumulation could be dangerous. Contact supplier if guidance is required.

**EWC Nr. 16 05 04***

## 14 TRANSPORT INFORMATION

**ADR/RID**

| | | | |
|---|---|---|---|
| Class | 2 | Classification Code | 2F |

**UN number and proper shipping name**

UN 1035 Ethane

UN 1035 Ethane

| | | | |
|---|---|---|---|
| Labels | 2.1 | Hazard number | 23 |
| Packing Instruction | P200 | | |

**IMDG**

Class 2.1

**UN number and proper shipping name**

UN 1035 Ethane

| | |
|---|---|
| Labels | 2.1 |
| Packing Instruction | P200 |
| EmS | FD,SU |

**IATA**

Class 2.1

**UN number and proper shipping name**

UN 1035 Ethane

| | |
|---|---|
| Labels | 2.1 |
| Packing Instruction | P200 |

**Other transport information**

Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers ensure that they are firmly secured. Ensure that the cylinder valve is closed and not leaking. Ensure that the valve outlet cap nut or plug (where provided) is correctly fitted. Ensure that the valve protection device (where provided) is correctly fitted. Ensure adequate ventilation. Ensure compliance with applicable regulations.

## 15 REGULATORY INFORMATION

**Further national regulations**

Pressure Vessel Regulation

Gefahrstoffverordnung (GefStoffV)

Technische Regeln für Gefahrstoffe (TRGS)

Regulations for the prevention of industrial accidents

**Water pollution class**

Not polluting to waters according to VwVwS from 17.05.99.

## 16 OTHER INFORMATION

Ensure all national/local regulations are observed. Ensure operators understand the flammability hazard. The hazard of asphyxiation is often overlooked and must be stressed during operator training. Before using this product in any new process or experiment, a thorough material compatibility and safety study should be carried out.

**Advice**

Whilst proper care has been taken in the preparation of this document, no liability for injury or damage resulting from its use can be accepted. Details given in this document are believed to be correct at the time of going to press.

**Further information**

Hommel: Handbook of dangerous goods

Kühn-Birett: Merkblätter gefährliche Arbeitsstoffe

Linde safety advice

THE LINDE GROUP Linde

# Safety data sheet
# Ethylene

| | | | | |
|---|---|---|---|---|
| Creation date : | 28.01.2005 | Version : 6.0 | DE / E | SDS No. : 055a |
| Revision date : | 04.01.2011 | | | page 1 / 3 |

## 1 IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY

**Product name**
Ethylene
EC No (from EINECS): 200-815-3
CAS No: 74-85-1
Index-Nr. 601-010-00-3
**Chemical formula** $C2H4$
**REACH Registration number**:
Not available.
**Known uses**
Not known.
**Company identification**
Linde AG, Linde Gas Division, Seitnerstraße 70, D-82049 Pullach
**E-Mail Address** Info@de.linde-gas.com
**Emergency phone numbers (24h):** 089-7446-0

## 2 HAZARDS IDENTIFICATION

**Classification of the substance or mixture**

**Classification acc. to Regulation (EC) No 1272/2008/EC (CLP/GHS)**
Press. Gas (Liquefied gas) - Contains gas under pressure; may explode if heated.
Flam. Gas 1 - Extremely flammable gas.
STOT SE 3 - May cause drowsiness or dizziness.

**Classification acc. to Directive 67/548/EEC & 1999/45/EC**
F+; R12 | R67
Extremely flammable.
Vapours may cause drowsiness and dizziness.
**Risk advice to man and the environment**
Compressed gas.
**Label Elements**

**- Labelling Pictograms**

**- Signal word**
Danger

**- Hazard Statements**

| | |
|---|---|
| H280 | Contains gas under pressure; may explode if heated. |
| H220 | Extremely flammable gas. |
| H336 | May cause drowsiness or dizziness. |

**- Precautionary Statements**

**Precautionary Statement Prevention**

| | |
|---|---|
| P210 | Keep away from heat/sparks/open flames/hot surfaces. - No smoking. |
| P260 | Do not breathe gas, vapours. |

**Precautionary Statement Reaction**

| | |
|---|---|
| P304+P340+P315 | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get immediate medical advise/attention. |
| P377 | Leaking gas fire: Do not extinguish, unless leakcan be stopped safely. |
| P381 | Eliminate all ignition sources if safe to do so. |

**Precautionary Statement Storage**

| | |
|---|---|
| P403 | Store in a well-ventilated place. |

**Precautionary Statement Disposal**
None.

## 3 COMPOSITION/INFORMATION ON INGREDIENTS

**Substance/Preparation:** Substance.
**Components/Impurities**
Ethylene
**CAS No:** 74-85-1
**Index-Nr.**: 601-010-00-3
**EC No (from EINECS):** 200-815-3
**REACH Registration number**:
Not available.
Contains no other components or impurities which will influence the classification of the product.

## 4 FIRST AID MEASURES

**Inhalation**
In high concentrations may cause asphyxiation. Symptoms may include loss of mobility/consciousness. Victim may not be aware of asphyxiation. In low concentrations may cause narcotic effects. Symptoms may include dizziness, headache, nausea and loss of co-ordination. Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.
**Ingestion**
Ingestion is not considered a potential route of exposure.

## 5 FIRE FIGHTING MEASURES

**Specific hazards**
Exposure to fire may cause containers to rupture/explode.
**Hazardous combustion products**
Incomplete combustion may form carbon monoxide.
**Suitable extinguishing media**
All known extinguishants can be used.
**Specific methods**
If possible, stop flow of product. Move container away or cool with water from a protected position. Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.
**Special protective equipment for fire fighters**
In confined space use self-contained breathing apparatus.

## 6 ACCIDENTAL RELEASE MEASURES

**Personal precautions**
Wear self-contained breathing apparatus when entering area unless atmosphere is proved to be safe. Evacuate area. Ensure adequate air ventilation. Eliminate ignition sources.
**Environmental precautions**
Try to stop release. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.
**Clean up methods**
Ventilate area.

THE LINDE GROUP — Linde

# Safety data sheet
# Ethylene

| | | | | |
|---|---|---|---|---|
| Creation date : | 28.01.2005 | Version : 6.0 | DE / E | SDS No. : 055a |
| Revision date : | 04.01.2011 | | | page 2 / 3 |

## 7 HANDLING AND STORAGE

**Handling**
Ensure equipment is adequately earthed. Suck back of water into the container must be prevented. Purge air from system before introducing gas. Do not allow backfeed into the container. Use only properly specified equipment which is suitable for this product, its supply pressure and temperature. Contact your gas supplier if in doubt. Keep away from ignition sources (including static discharges). Refer to supplier's handling instructions.
**Storage**
Secure cylinders to prevent them falling. Segregate from oxidant gases and other oxidants in store. Keep container below 50°C in a well ventilated place. Observe "Technische Regeln Druckgase (TRG) 280 Ziffer 5"

## 8 EXPOSURE CONTROLS/PERSONAL PROTECTION

**Personal protection**
Ensure adequate ventilation. Do not smoke while handling product. Carry working gloves and protection shoes while handling gas cylinders.

## 9 PHYSICAL AND CHEMICAL PROPERTIES

**General information**
**Appearance/Colour:** Colourless gas.
**Odour:** Poor warning properties at low concentrations. Sweetish.
**Important information on environment, health and safety**
**Molecular weight:** 28 g/mol
**Melting point:** -169 °C
**Boiling point:** -103 °C
**Critical temperature:** 9,5 °C
**Autoignition temperature:** 425 °C
**Flammability range:** 2,3 %(V) - 34 %(V)
**Relative density, gas:** 1
**Relative density, liquid:** 0,57
**Vapour Pressure 20 °C:** Not applicable.
**Solubility mg/l water:** No reliable data available.
**Other data**
Gas/vapour heavier than air. May accumulate in confined spaces, particularly at or below ground level.

## 10 STABILITY AND REACTIVITY

**Stability and reactivity**
May decompose violently at high temperature and/or pressure or in the presence of a catalyst Can form explosive mixture with air. May react violently with oxidants.

## 11 TOXICOLOGICAL INFORMATION

**Acute toxicity**
No known toxicological effects from this product.

## 12 ECOLOGICAL INFORMATION

**General**
No known ecological damage caused by this product.

## 13 DISPOSAL CONSIDERATIONS

**General**
Do not discharge into areas where there is a risk of forming an explosive mixture with air. Waste gas should be flared through a suitable burner with flash back arrestor. Do not discharge into any place where its accumulation could be dangerous. Contact supplier if guidance is required.
**EWC Nr. 16 05 04***

## 14 TRANSPORT INFORMATION

**ADR/RID**

| | | | |
|---|---|---|---|
| Class | 2 | Classification Code | 2F |

**UN number and proper shipping name**
UN 1962 Ethylene
UN 1962 Ethylene

| | | | |
|---|---|---|---|
| Labels | 2.1 | Hazard number | 23 |

**IMDG**

| | |
|---|---|
| Class | 2.1 |

**UN number and proper shipping name**
UN 1962 Ethylene

| | |
|---|---|
| Labels | 2.1 |
| Packing Instruction | P200 |
| EmS | FD,SU |

**IATA**

| | |
|---|---|
| Class | 2.1 |

**UN number and proper shipping name**
UN 1962 Ethylene

| | |
|---|---|
| Labels | 2.1 |
| Packing Instruction | P200 |

**Other transport information**
Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers ensure that they are firmly secured. Ensure that the cylinder valve is closed and not leaking. Ensure that the valve outlet cap nut or plug (where provided) is correctly fitted. Ensure that the valve protection device (where provided) is correctly fitted. Ensure adequate ventilation. Ensure compliance with applicable regulations.

## 15 REGULATORY INFORMATION

**Further national regulations**
Pressure Vessel Regulation
Gefahrstoffverordnung (GefStoffV)
Technische Regeln für Gefahrstoffe (TRGS)
Regulations for the prevention of industrial accidents
**Water pollution class**
Not polluting to waters according to VwVwS from 17.05.99.
**TA-Luft**
Not classified according to TA-Luft.

## 16 OTHER INFORMATION

Ensure all national/local regulations are observed. Ensure operators understand the flammability hazard. The hazard of asphyxiation is often overlooked and must be stressed during operator training. Before using this product in any new process or experiment, a thorough material compatibility and safety study should be carried out.
**Advice**
Whilst proper care has been taken in the preparation of this document, no liability for injury or damage resulting from its use can be accepted. Details given in this document are believed to be correct at the time of going to press.
**Further information**
Hommel: Handbook of dangerous goods

United Hydrogen
GROUP

# Material Safety Data Sheet: Hydrogen

| | |
|---|---|
| **Product Name:** Hydrogen | **CAS:** 1333-74-0 |
| Hydrogen, Compressed (D.O.T); Water Gas | **DOT I.D No.:** UN 1049 |
| **Chemical Name and Synonyms:** Hydrogen, Normal Hydrogen | **DOT Hazard Class:** Division 2.1 |
| **Formula:** $H_2$ | **Chemical Family:** Inorganic Flammable Gas |

## Health Hazard Data

### Time Weighted Average Exposure Limit:

Hydrogen is defined as a simple asphyxiant (ACGIH 1994-1995); OSHA 1993 PEL (8 Hr. TWA) = No Listing

### Symptoms of Exposure:

Inhalation: High concentrations of hydrogen so as to exclude an adequate supply of oxygen to the lungs causes dizziness, deeper breathing due to air hunger, possible nausea and eventual unconsciousness.

### Toxicological Properties:

Hydrogen is inactive biologically and essentially nontoxic; therefore, the major property is the exclusion of an adequate supply of oxygen to the lungs.

Hydrogen is not listed in the IARC, NTP or by OSHA as a carcinogen or potential carcinogen.

Persons in ill health where such illness would be aggravated by exposure to hydrogen should not be allowed to work with or handle this product.

| | |
|---|---|
| **Hazardous Mixtures of other Liquids, Solids or Gases:** Hydrogen is flammable over a very wide range in air. | |
| PHYSICAL DATA | |
| **Boiling Point:** -423°F (-252.8°C) | **Liquid Density at Boiling Point:** 4.43 lb/ft3 (70.96 kg/m3) |
| **Vapor Pressure** @ 70°F (21.1 °C) = Above the critical temperature of 399.8°F (-239.9°C) | **Gas Density at 70°F. 1 atm** .0052 |
| **Solubility in Water:** Very slightly | **Freezing Point:** -434.6°F (-259.2°C) |
| **Evaporation Rate:** N/A (Gas) | **Specific Gravity (AIR=1)** @ 70F (21.1°C) = .069 |
| **Appearance and Odor:** Colorless, odorless gas | |

## Fire and Explosion Hazard Data

| | | |
|---|---|---|
| **Flash Point (Method used):** N/A Gas | **Auto Ignition Temperature:** 1058°F (570°C) | **Flammable Limits % by Volume:** LEL 4 UEL 74.5 |
| **Extinguishing Media:** Water, carbon dioxide, dry chemical | | **Electrical Classification:** Class 1, Group B |
| **Special Fire fighting Procedures:** If possible, stop the flow of hydrogen. Cool surrounding containers with water spray. Hydrogen burns with an almost invisible flame of relatively low thermal radiation. | | |
| **Unusual Fire and Explosion Hazards:** Hydrogen is very light and rises very rapidly in air. Should a hydrogen fire be extinguished and the flow of gas continue, increase ventilation to prevent an explosion hazard, particularly in the upper portions. | | |

## Reactivity Data

**Stability:** Stable

**Incompatibility (Materials to Avoid):** Oxidizers

**Hazardous Decomposition Products:** None

**Hazardous Polymerization:** Will not occur

**Conditions to Avoid** None

## Spill or Leak Procedures

**Steps to be taken in case material is released or spilled:**

Evacuate all personnel from affected area. Use appropriate protective equipment. If leak is in user's equipment, be certain to purge piping with an inert gas prior to attempting repairs. If leak is in container or container valve, contact your closest supplier location or call the emergency telephone number listed herein.

**Waste disposal methods:**

Do not attempt to dispose of waste or unused quantities. Return in the shipping container properly labeled, with any valve outlet plugs or caps secured and valve protection cap in place to your supplier. For emergency disposal assistance, contact your closest supplier location or call the emergency telephone number listed herein.

## Special Protection Information

**Respiratory Protection (Specify type):** Positive pressure air line with mask or self-contained breathing apparatus should be available for emergency use.

**Ventilation:** Hood with forced ventilation

**Local Exhaust:** To prevent accumulation above the LEL

**Mechanical (Gen.):** In accordance with electrical codes

**Protective Gloves:** Plastic or rubber

**Eye Protection:** Safety goggles or glasses

**Other Protective Equipment:** Safety shoes, safety shower

## Special Precautions

**Special Labeling Information:**

DOT Shipping Name: Hydrogen, Compressed

DOT Hazard Class: Division 2.1

DOT Shipping Label: Flammable Gas

I.D. No.: UN 1049

**Special Handling Recommendation:**

Use only in well-ventilated areas. Valve protection caps must remain in place unless container is secured with valve outlet piped to use point. Do not drag, slide or roll cylinders. Use a suitable hand truck for cylinder movement. Use a pressure reducing regulator when connecting cylinder to lower pressure (<3,000 psig) piping or systems. Do not heat cylinder by any means to increase the discharge rate of product from the cylinder. Use a check valve or trap in the discharge line to prevent hazardous back flow into the cylinder. For additional handling recommendations, consult Compressed Gas Association's Pamphlets G-5, P-1, P-14, and Safety Bulletin SB-2.

**Special Storage Recommendations:**

Protect cylinders from physical damage. Store in cool, dry, well-ventilated area of I noncombustible construction away from heavily trafficked areas and emergency exits. Do not allow the temperature where cylinders are stored to exceed 125F (52C). Cylinders should be stored upright and firmly secured to prevent falling or being knocked over. Full and empty cylinders should be segregated. Use a "first in -first out" inventory system to prevent full cylinders being stored for excessive periods of time. Post "No Smoking or Open Flames" signs in the storage or use area. There should be no sources of ignition in the storage or use area. For additional storage recommendations, consult Compressed Gas Association's Pamphlets G-5, P-1, P-14, and Safety Bulletin SB-2.

**Other Recommendations or Precautions:**

Earth-ground and bond all lines and equipment associated with the hydrogen system. Electrical equipment should be non-sparking or explosion proof. Compressed gas cylinders should not be refilled except by qualified producers of compressed gases. Shipment of a compressed gas cylinder which has not been filled by the owner or with his (written) consent is a violation of Federal Law (49CFR).

**Special Packaging Recommendations:**

Hydrogen is non-corrosive and may be used with any common structural material.

# MSDS

**MATERIAL SAFETY DATA SHEET**

ZEOLYST INTERNATIONAL

*Trade Name:* **CBV2314**

**ZEOLITE AMMONIUM ZSM-5 POWDER**

*Date Prepared:* **03/14/06** *Page:* **1 of 4**

## 1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

| | |
|---|---|
| *Product name:* | **CBV2314** |
| *Product description:* | **ZEOLITE AMMONIUM ZSM-5 POWDER** |
| *Manufacturer:* | **Zeolyst International**<br>**P. O. Box 830**<br>**Valley Forge, PA 19482 USA** |
| *Telephone:* | **610-651-4200** |
| *In case of emergency call:* | **610-651-4200** |
| *For transportation emergency Call CHEMTREC:* | **800-424-9300** |

## 2. COMPOSITION/INFORMATION ON INGREDIENTS

| *Chemical and Common Name* | *CAS Registry Number* | *Wt. %* | *OSHA PEL* | *ACGIH TLV* |
|---|---|---|---|---|
| **Zeolite** | **1318-02-1** | **100%** | **15mg/m$^3$ total dust**<br>**5mg/m$^3$ respirable** | **10 mg/m$^3$**<br>**3 mg/m$^3$ respirable** |

**(Particulates Not Otherwise Regulated)**

## 3. HAZARDS IDENTIFICATION

| | |
|---|---|
| *Emergency Overview*: | **White, odorless, powder. Causes respiratory irritation. Causes mild eye irritation. May cause skin irritation. Ammonia released on contact with strong bases. Noncombustible. Ammonia or nitrogen oxides may be released at high temperatures.** |
| *Eye contact:* | **Causes mild eye irritation.** |
| *Skin contact:* | **Prolonged or repeated contact may dry skin and cause irritation.** |
| *Inhalation:* | **Causes irritation.** |
| *Ingestion:* | **No known hazards. Inedible.** |
| *Chronic hazards:* | **No known hazards.** |
| *Physical hazards:* | **Absorbs water from air and fluids. Generates heat when it absorbs water.** |

## 4. FIRST AID MEASURES

| | |
|---|---|
| *Eye:* | **In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention if irritation persists.** |
| *Skin:* | **In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if irritation develops** |

**and persists. Wash clothing before reuse. Thoroughly clean shoes before reuse.**

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

*Ingestion:* **Not applicable.**

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## 5. FIRE FIGHTING MEASURES

*Flammable limits:* **This material is noncombustible.**

*Extinguishing Media:* **This material is compatible with all extinguishing media.** *Hazards to fire-fighters:* **Ammonia or nitrogen oxides may be released at high temperatures.**

*Fire-fighting equipment:* **The following protective equipment for fire fighters is recommended when this material is present in the area of a fire: self-contained breathing apparatus (SCBA), chemical goggles, body-covering protective clothing, chemical resistant gloves, and rubber boots.**

---

## 6. ACCIDENTAL RELEASE MEASURES

*Personal protection:* **Wear safety goggles, body-covering protective clothing, chemical resistant gloves, and rubber boots, NIOSH-approved dust respirator where dust occurs. See section 8.**

*Environmental Hazards:* **Sinks in water. No know environmental hazards.**

*Small spill cleanup:* **Carefully shovel or sweep up spilled material and place in suitable container. Avoid generating dust. Use appropriate Personal Protective Equipment (PPE). See section 8.**

*Large spill cleanup:* **Keep unnecessary people away; isolate hazard area and deny entry. Do not touch or walk through spilled material. Carefully shovel or sweep up spilled material and place in suitable container. Avoid generating dust. Use appropriate Personal Protective Equipment (PPE). See section 8.**

*CERCLA RQ:* **There is no CERCLA Reportable Quantity for this material. If a spill goes off site, notification of state and local authorities is recommended.**

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## 7. HANDLING AND STORAGE

| | |
|---|---|
| *Handling:* | **Avoid contact with eyes, skin and clothing. Avoid breathing dust. Keep container closed. Promptly clean up spills. Wash thoroughly after handling.** |
| *Storage:* | **Keep containers closed. Store separated from strong bases in original containers or clean metal, plastic, or fiber containers.** |

*Trade Name:* **CBV2314**

**ZEOLITE AMMONIUM ZSM5 POWDER**

*Date*

*Prepared:* **03/14/06** *Page:***3 of 4**

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

| | |
|---|---|
| *Engineering controls:* | **Use with adequate ventilation. Safety shower and eyewash fountain should be within direct access.** |
| *Respiratory protection:* | **Use a NIOSH-approved dust respirator where dust occurs. Observe OSHA regulations for respirator use (29 C.F.R. §1910.134)** |
| *Skin protection:* | **Wear body-covering protective clothing and gloves.** |
| *Eye protection:* | **Wear safety goggles.** |

## 9. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|---|---|
| *Appearance:* | **White powder.** |
| *Odor:* | **Odorless.** |
| *pH:* | **Not applicable.** |
| *Specific Gravity:* | **>1.** |
| *Solubility in water:* | **Negligible.** |

## 10. STABILITY AND REACTIVITY

| | |
|---|---|
| *Stability:* | **This material is stable.** |
| *Conditions to avoid:* | **None.** |
| *Materials to avoid:* | **Ammonia may be released on contact with strong bases.** |
| *Hazardous decomposition products:* | **Ammonia, nitrogen oxides.** |

## 11. TOXICOLOGICAL INFORMATION

*Acute Data:* **When tested for primary irritation potential, similar materials caused mild eye irritation and were slightly irritating or non-irritating to the skin. Human experience with similar materials indicates that prolonged or repeated contact may dry skin and cause irritation. This material has not been tested for acute inhalation toxicity. It contains fine particles which can cause respiratory irritation. The acute oral toxicity of this material has not been tested. There are currently no reports of human toxicity for ingested zeolite.**

*Subchronic Data:* **This material has not been tested for subchronic toxicity potential.**

*Special Studies:* **This material has not been tested for chronic inhalation toxicity. Zeolite Beta is not listed by NTP, IARC, or OSHA as a carcinogen.**

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| | |
|---|---|
| Health | 2 |
| Fire | 3 |
| Reactivity | 0 |
| Personal Protection | J |

# Material Safety Data Sheet
# m-Xylene MSDS

## Section 1: Chemical Product and Company Identification

**Product Name:** m-Xylene

**Catalog Codes:** SLX1066

**CAS#:** 108-38-3

**RTECS:** ZE2275000

**TSCA:** TSCA 8(b) inventory: m-Xylene

**CI#:** Not applicable.

**Synonym:** m-Methyltoluene

**Chemical Name:** 1,3-Dimethylbenzene

**Chemical Formula:** C6H4(CH3)2

**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 |
|---|---|---|
| {m-}Xylene | 108-38-3 | 100 |

**Toxicological Data on Ingredients:** m-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 14100 mg/kg [Rabbit.].

## Section 3: Hazards Identification

**Potential Acute Health Effects:**
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. 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 eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

## Section 4: First Aid Measures

**Eye Contact:** Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

**Skin Contact:**
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

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

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

**Serious Inhalation:** Not available.

**Ingestion:**
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

**Serious Ingestion:** Not available.

## Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 527°C (980.6°F)

**Flash Points:** CLOSED CUP: 25°C (77°F). OPEN CUP: 28.9°C (84°F) (Cleveland).

**Flammable Limits:** LOWER: 1.1% UPPER: 7%

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

**Fire Hazards in Presence of Various Substances:** Highly flammable in presence of open flames and sparks, 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, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use 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:**
Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

**Special Remarks on Explosion Hazards:** Not available.

## Section 6: Accidental Release Measures

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**
Flammable liquid, insoluble in water. 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. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

## Section 7: Handling and Storage

**Precautions:**
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. 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.

**Storage:**
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

## Section 8: Exposure Controls/Personal Protection

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

**Personal Protection:** Splash goggles. Lab coat. Gloves.

**Personal Protection in Case of a Large Spill:**
Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

**Exposure Limits:**
TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIHConsult local authorities for acceptable exposure limits.

## Section 9: Physical and Chemical Properties

**Physical state and appearance:** Liquid. (Liquid.)

**Odor:** Not available.

**Taste:** Not available.

**Molecular Weight:** 106.17 g/mole

**Color:** Colorless.

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

**Boiling Point:** 139.3°C (282.7°F)

**Melting Point:** -47.87°C (-54.2°F)

**Critical Temperature:** Not available.

**Specific Gravity:** 0.86 (Water = 1)

**Vapor Pressure:** 6 mm of Hg (@ 20°C)

**Vapor Density:** 3.7 (Air = 1)

**Volatility:** Not available.

**Odor Threshold:** 0.62 ppm

**Water/Oil Dist. Coeff.:** Not available.

**Ionicity (in Water):** Not available.

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

**Solubility:**
Easily soluble in methanol, diethyl ether. Insoluble in cold water, hot water.

## Section 10: Stability and Reactivity Data

**Stability:** The product is stable.

**Instability Temperature:** Not available.

**Conditions of Instability:** Not available.

**Incompatibility with various substances:** Reactive with oxidizing agents.

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

**Special Remarks on Reactivity:** Not available.

**Special Remarks on Corrosivity:** Not available.

**Polymerization:** No.

## Section 11: Toxicological Information

**Routes of Entry:** Eye contact.

**Toxicity to Animals:**
Acute oral toxicity (LD50): 5000 mg/kg [Rat.]. Acute dermal toxicity (LD50): 14100 mg/kg [Rabbit.].

**Chronic Effects on Humans:** The substance is toxic to blood, kidneys, the nervous system, liver.

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

**Special Remarks on Toxicity to Animals:** Not available.

**Special Remarks on Chronic Effects on Humans:**
0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

**Special Remarks on other Toxic Effects on Humans:** Material is irritating to mucous membranes and upper respiratory tract.

## Section 12: Ecological Information

**Ecotoxicity:** Not available.

**BOD5 and COD:** Not available.

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

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

**Special Remarks on the Products of Biodegradation:** Not available.

## Section 13: Disposal Considerations

**Waste Disposal:**

## Section 14: Transport Information

**DOT Classification:** Class 3: Flammable liquid.

**Identification:** : Xylene : UN1307 PG: III

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

## Section 15: Other Regulatory Information

**Federal and State Regulations:**
Pennsylvania RTK: m-Xylene Massachusetts RTK: m-Xylene TSCA 8(b) inventory: m-Xylene SARA 313 toxic chemical notification and release reporting: m-Xylene CERCLA: Hazardous substances.: m-Xylene

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

**Other Classifications:**

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

**DSCL (EEC):**
R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes.

**HMIS (U.S.A.):**

**Health Hazard:** 2

**Fire Hazard:** 3

**Reactivity:** 0

**Personal Protection:** j

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

**Health:** 2

**Flammability:** 3

**Reactivity:** 0

**Specific hazard:**

**Protective Equipment:**
Gloves. Lab coat. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

## Section 16: Other Information

**References:**
-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

**Other Special Considerations:** Not available.

**Created:** 10/10/2005 08:33 PM

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

Manufactured for

**INDUSTRIAL SCIENTIFIC CORPORATION**

1001 Oakdale Road
Oakdale, PA 15071-1500

Phone (412) 788-4353
TOLL-FREE 800-DETECTS
Fax (412) 788-8353

# MATERIAL SAFETY DATA SHEET

*Prepared to U.S. OSHA, CMA, ANSI and Canadian WHMIS Standards*

## 1. PRODUCT IDENTIFICATION

### CHEMICAL NAME; CLASS: METHANE

**SYNONYMS:** Methyl Hydride; Marsh Gas
**CHEMICAL FAMILY:** Alkane (hydrocarbon)
**FORMULA:** $CH_4$

**Document Number:** 50006 (Replaces ISC MSDS No.1810-2312, 1810-4778)

**Note:** This Material Safety Data Sheet is for Methane supplied in cylinders with 33 cubic feet (935 liters) or less gas capacity (DOT 39 cylinders). For Methane in large cylinders refer to Document Number 10060

| | |
|---|---|
| **PRODUCT USE:** | Calibration of Monitoring and Research Equipment |
| **SUPPLIER/MANUFACTURER'S NAME:** | CALGAZ |
| **ADDRESS:** | 821 Chesapeake Drive<br>Cambridge, MD 21613 |
| **EMERGENCY PHONE:** | CHEMTREC: 1-800-424-9300 |
| **BUSINESS PHONE:** | 1-410-228-6400 |
| General MSDS Information: | 1-713/868-0440 |
| Fax on Demand: | 1-800/231-1366 |

## 2. COMPOSITION and INFORMATION ON INGREDIENTS

| CHEMICAL NAME | CAS # | mole % | EXPOSURE LIMITS IN AIR | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | ACGIH-TLV | | OSHA-TLV | | NIOSH | OTHER |
| | | | TWA ppm | STEL ppm | TWA ppm | STEL ppm | IDLH ppm | ppm |
| Methane | 74-82-8 | > 98% | There are no specific exposure limits for Methane. Methane is a simple asphyxiant (SA). Oxygen levels should be maintained above 19.5%. | | | | | |
| Maximum Impurities | | < 2.0% | None of the trace impurities in this product contribute significantly to the hazards associated with the product. All hazard information pertinent to this product has been provided in this Material Safety Data Sheet, per the requirements of the OSHA Hazard Communication Standard (29 CFR 1910.1200) and State equivalents standards. | | | | | |

NE = Not Established. See Section 16 for Definitions of Terms Used.

NOTE (1): ALL WHMIS required information is included in appropriate sections based on the ANSI Z400.1-1998 format. This product has been classified in accordance with the hazard criteria of the CPR and the MSDS contains all the information required by the CPR.

## 3. HAZARD IDENTIFICATION

**EMERGENCY OVERVIEW**: This product is a colorless, flammable gas. The main health hazard associated with overexposure to this gas is asphyxiation, by displacement of oxygen. The gas poses a serious fire hazard when accidentally released. Flame or high temperature impinging on a localized area of the cylinder of this product can cause the cylinder to burst or rupture without activating the cylinder's relief devices. The gas is lighter than air, and may spread long distances. Distant ignition and flashback are possible. Provide adequate fire protection during emergency response situations.

**SYMPTOMS OF OVER-EXPOSURE BY ROUTE OF EXPOSURE**: The most significant route of over-exposure for this product is by inhalation.

**INHALATION**: Due to the small size of an individual cylinder of this product, no unusual health effects from exposure to the product are anticipated under routine circumstances of use. If this product is released in a small, poorly ventilated area (i.e. an enclosed or confined space), an oxygen-deficient environment may occur. It should be noted that before suffocation could occur, the lower flammability limit of Methane in air would be exceeded; possibly causing an oxygen-deficient and explosive atmosphere. Individuals breathing an oxygen deficient atmosphere may experience symptoms which include headaches, ringing in ears, dizziness, drowsiness, unconsciousness, nausea, vomiting, and depression of all the senses. Under some circumstances of over-exposure, death may occur. The following effects associated with various levels of oxygen are as follows:

| OXYGEN CONCENTRATION | SYMPTOM OF EXPOSURE |
|---|---|
| 12-16% Oxygen: | Breathing and pulse rate increased, muscular coordination slightly disturbed. |
| 10-14% Oxygen: | Emotional upset, abnormal fatigue, disturbed respiration. |
| 6-10% Oxygen: | Nausea and vomiting, collapse or loss of consciousness. |
| Below 6%: | Convulsive movements, possible respiratory collapse, and death. |

**HEALTH EFFECTS OR RISKS FROM EXPOSURE: An Explanation in Lay Terms**. Over-exposure to this gas mixture may cause the following health effects:

**ACUTE**: Due to the small size of the individual cylinder of this product, no unusual health effects from exposure to the product are anticipated under routine circumstances of use. The most significant hazard associated with this product is inhalation of oxygen-deficient atmospheres. Symptoms of oxygen deficiency include respiratory difficulty, ringing in ears, headaches, shortness of breath, wheezing, headache, dizziness, indigestion, nausea, and, at high concentrations, unconsciousness or death may occur. The skin of a victim of over-exposure may have a blue color.

**CHRONIC**: Chronic exposure to oxygen-deficient atmospheres (below 18% oxygen in air) may effect the heart and nervous system.

**TARGET ORGANS**: ACUTE: Respiratory system. CHRONIC: Heart, central nervous system.

**HAZARDOUS MATERIAL IDENTIFICATION SYSTEM**

| | |
|---|---|
| **HEALTH HAZARD** (BLUE) | 1 |
| **FLAMMABILITY HAZARD** (RED) | 4 |
| **PHYSICAL HAZARD** (YELLOW) | 0 |

PROTECTIVE EQUIPMENT

| EYES | RESPIRATORY | HANDS | BODY |
|---|---|---|---|
| See Section 8 | | | |

For Routine Industrial Use and Handling Applications

## 4. FIRST-AID MEASURES

**RESCUERS SHOULD NOT ATTEMPT TO RETRIEVE VICTIMS OF OVER-EXPOSURE TO THIS PRODUCT WITHOUT ADEQUATE PERSONAL PROTECTIVE EQUIPMENT. At a minimum, Self-Contained Breathing Apparatus and Fire-Retardant Personal Protective equipment should be worn. Adequate fire protection must be provided during rescue situations.**

No unusual health effects are anticipated after exposure to this product, due to the small cylinder size. If any adverse symptom develops after over-exposure to this product, remove victim(s) to fresh air, as quickly as possible. Only trained personnel should administer supplemental oxygen and/or cardio-pulmonary resuscitation, if necessary. Victim(s) who experience any adverse effect after over-exposure to this product must be taken for medical attention. Rescuers should be taken for medical attention, if necessary. Take copy of label and MSDS to physician or other health professional with victim(s).

**THERMAL BURNS**: In the event personnel are burned as a result of a Hydrogen release, if burns are first degree or second degree with closed blisters, flush area with cold water until pain subsides. Apply loose, moist, sterile dressings, and bandage. Treat for shock. If burns are second degree with open blisters or third degree, apply loose, dry, sterile dressings and bandage. Treat for shock. Transport victim immediately to hospital or emergency center. Burns over an area of 20% or more of body are life-threatening, medical attention should be immediately sought.

**MEDICAL CONDITIONS AGGRAVATED BY EXPOSURE**: None known.

**RECOMMENDATIONS TO PHYSICIANS**: Treat symptoms and reduce over-exposure.

## 5. FIRE-FIGHTING MEASURES

**FLASH POINT:** -187.7°C (-306°F)

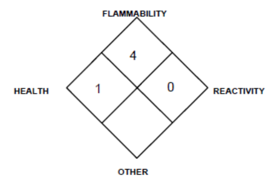
**AUTOIGNITION TEMPERATURE:** 650°C (1202°F)

**FLAMMABLE LIMITS (in air by volume, %):**

Lower (LEL): 5.0%

Upper (UEL): 15.0%

**NFPA RATING**




**FIRE EXTINGUISHING MATERIALS**: Extinguish Methane fires by shutting-off the source of the gas. Use water spray to cool fire-exposed containers, structures, and equipment.

**UNUSUAL FIRE AND EXPLOSION HAZARDS**: When involved in a fire, this material may decompose and produce toxic gases including carbon monoxide and carbon dioxide.

**DANGER!** Fires impinging (direct flame) on the outside surface of unprotected cylinders of this product can be very dangerous. Exposure to fire could cause a catastrophic failure of the cylinder releasing the contents into a fireball and explosion of released gas. The resulting fire and explosion can result in severe equipment damage and personnel injury or death over a large area around the cylinder. For massive fires in large areas, use unmanned hose holder or monitor nozzles; if this is not possible, withdraw from area and allow fire to burn.

Explosion Sensitivity to Mechanical Impact: Not sensitive.

Explosion Sensitivity to Static Discharge: Static discharge may cause this product to ignite explosively, if released.

**SPECIAL FIRE-FIGHTING PROCEDURES**: Structural fire-fighters must wear Self-Contained Breathing Apparatus and full protective equipment. Because of the potential for a fire, evacuation of non-emergency personnel is essential. If water is not available for cooling or protection of cylinder exposures, evacuate the area. The North American Emergency Response Guidebook (Guide #115) recommends 0.5 miles.

## 6. ACCIDENTAL RELEASE MEASURES

**LEAK RESPONSE**: **LEAK RESPONSE**: Due to the small size and content of the cylinder, an accidental release of this product presents significantly less risk of a flammability and Oxygen deficient environment and other safety hazards than a similar release from a larger cylinder. However, as with any chemical release, extreme caution must be used during emergency response procedures. In the event of a release in which the atmosphere is unknown, and in which other chemicals are potentially involved, evacuate immediate area. Uncontrolled releases should be responded to by trained personnel using pre-planned procedures. Proper protective equipment should be used. In case of a gas release, clear the affected area, protect people, and respond with trained personnel.

Eliminate any possible sources of ignition, and provide maximum explosion-proof ventilation. If the gas is leaking from cylinder contact the supplier. Adequate fire protection must be provided. Use only non-sparking tools and equipment during the response. Allow the gas, which is lighter than air to dissipate. If necessary, monitor the surrounding area (and the original area of the release) for oxygen. Oxygen levels must be above 19.5% before non-emergency personnel are allowed to re-enter area. Combustible gas concentration must be below 10% of the LEL (5.0%) prior to entry.

If leaking incidentally from the cylinder, contact your supplier.

**THIS IS AN EXTREMELY FLAMMABLE GAS.** Protection of all personnel and the area must be maintained.

## 7. HANDLING and USE

**WORK PRACTICES AND HYGIENE PRACTICES**: Be aware of any signs of dizziness or fatigue; exposures to fatal concentrations of this product could occur without any significant warning symptoms. Use non-sparking tools when working with Methane.

**STORAGE AND HANDLING PRACTICES**: Cylinders should be firmly secured to prevent falling or being knocked-over. Cylinders must be protected from the environment, and preferably kept at room temperature approximately 21°C, 70°F. Cylinders should be stored in dry, well-ventilated areas away from sources of heat, ignition and direct sunlight. Keep storage area clear of materials which can burn. Protect cylinders against physical damage.

Cylinders should be separated from oxygen cylinders, or other oxidizers, by a minimum distance of 20 ft., or by a barrier of non-combustible material at least 5 ft. high, having a fire-resistance rating of at least 0.5 hours. Isolate from other incompatible chemicals (refer to Section 10, Stability and Reactivity).

Storage areas must meet national electrical codes for Class 1 Hazardous Areas. Post "No Smoking or Open Flames" signs in storage or use areas. Consider installation of leak detection for combustible gas levels and alarm for storage and use areas. Have appropriate extinguishing equipment in the storage area (i.e. sprinkler system, portable fire extinguishers).

Full and empty cylinders should be segregated. Use a first-in, first-out inventory system to prevent full containers from being stored for long periods of time. These cylinders are not refillable. **WARNING! Do not refill DOT 39 cylinders. To do so may cause personal injury or property damage.**

**SPECIAL PRECAUTIONS FOR HANDLING GAS CYLINDERS: WARNING!** Compressed gases can present significantly safety hazards. During cylinder use, use equipment designed for these specific cylinders. Ensure all lines and equipment are rated for proper service pressure.

**PROTECTIVE PRACTICES DURING MAINTENANCE OF CONTAMINATED EQUIPMENT**: Follow practices indicated in Section 6 (Accidental Release Measures). Make certain application equipment is locked and tagged-out safely. Purge gas handling equipment with inert gas (i.e. nitrogen) before attempting repairs. Always use product in areas where adequate ventilation is provided.

## 8. EXPOSURE CONTROLS - PERSONAL PROTECTION

**VENTILATION AND ENGINEERING CONTROLS**: No special ventilation systems or engineering controls are needed under normal circumstances of use. As with all chemicals, use this product in well-ventilated areas. Monitoring may be appropriate to detect if the level of Methane exceeds 10% of the LEL (5%).

**RESPIRATORY PROTECTION**: No special respiratory protection is required under normal circumstances of use. Use supplied air respiratory protection if Oxygen levels are below 19.5%, or unknown, during emergency response to a release of this product. If respiratory protection is needed, use only protection authorized in the U.S. Federal OSHA Standard (29 CFR 1910.134), applicable U.S. State regulations, or the Canadian CSA Standard Z94.4-93 and applicable standards of Canadian Provinces. Oxygen levels below 19.16.33% are considered IDLH by OSHA. In such atmospheres, use of a full-facepiece pressure/demand SCBA or a full facepiece, supplied air respirator with auxiliary self-contained air supply is required under OSHA's Respiratory Protection Standard (1910.134-1998).

## 8. EXPOSURE CONTROLS - PERSONAL PROTECTION (CONTINUED)

**EYE PROTECTION**: Safety glasses. If necessary, refer to U.S. OSHA 29 CFR 1910.133 or appropriate Canadian Standards.
**HAND PROTECTION**: No special protection is needed under normal circumstances of use. If necessary, refer to U.S. OSHA 29 CFR 1910.138 or appropriate Standards of Canada.
**BODY PROTECTION**: No special protection is needed under normal circumstances of use. If a hazard of injury to the feet exists due to falling objects, rolling objects, where objects may pierce the soles of the feet or where employee's feet may be exposed to electrical hazards, use foot protection, as described in U.S. OSHA 29 CFR 1910.136.

## 9. PHYSICAL and CHEMICAL PROPERTIES

**GAS DENSITY @ 60°F (15.6°C) and 1 atm:** 0.042 35 lb/ft$^3$
**BOILING POINT**: -161°C (-258.7°F)
**FREEZING/MELTING POINT (@ 10 psig)**: -182°C (-296.5°F)
**SPECIFIC GRAVITY (air = 1) @ 70°F (21.1°C):** 0.555
**pH**: Not applicable.
**SOLUBILITY IN WATER vol/vol at 100°F (37.8°C):** Very slight.
**MOLECULAR WEIGHT:** 16.042
**EVAPORATION RATE (nBuAc = 1):** Not applicable.
**EXPANSION RATIO:** Not applicable.
**ODOR THRESHOLD**: Not determined.
**SPECIFIC VOLUME (ft$^3$/lb):** 23.6
**VAPOR PRESSURE @ 70°F (21.1°C) (psig)**: Not applicable.
**COEFFICIENT WATER/OIL DISTRIBUTION**: Not applicable.
**APPEARANCE, ODOR AND COLOR**: Colorless, odorless gas.
**HOW TO DETECT THIS SUBSTANCE (warning properties):** There are no distinct warning properties of this gas. In terms of leak detection, fittings and joints can be painted with a soap solution to detect leaks, which will be indicated by a bubble formation.
**NOTE**: This gas is lighter than air and must not be allowed to accumulate in elevated locations

## 10. STABILITY and REACTIVITY

**STABILITY**: Stable under conditions of normal temperature and pressure.
**DECOMPOSITION PRODUCTS:** When ignited in the presence of air, this gas will burn to produce carbon monoxide, carbon dioxide.
**MATERIALS WITH WHICH SUBSTANCE IS INCOMPATIBLE**: Strong oxidizers (i.e. chlorine, bromine pentafluoride, oxygen, oxygen difluoride, and nitrogen trifluoride).
**HAZARDOUS POLYMERIZATION**: Will not occur.
**CONDITIONS TO AVOID**: Contact with incompatible materials and exposure to heat, sparks and other sources of ignition. Cylinders exposed to high temperatures or direct flame can rupture or burst.

## 11. TOXICOLOGICAL INFORMATION

**TOXICITY DATA**: There is no specific toxicology data for Methane. Methane is a simple asphyxiant, which acts to displace oxygen in the environment.
**SUSPECTED CANCER AGENT**: Methane is not found on the following lists: FEDERAL OSHA Z LIST, NTP, IARC, CAL/OSHA; therefore is not considered to be, nor suspected to be a cancer-causing agent by these agencies.
**IRRITANCY OF PRODUCT**: Methane is not irritating; however, contact with rapidly expanding gases can cause frostbite to exposed tissue.
**SENSITIZATION OF PRODUCT**: Methane is not a sensitizer.
**REPRODUCTIVE TOXICITY INFORMATION**: Listed below is information concerning the effects of Methane on the human reproductive system.

Mutagenicity: No mutagenicity effects have been described for Methane
Embryotoxicity: No embryotoxic effects have been described for Methane.
Teratogenicity: No teratogenicity effects have been described for Methane.
Reproductive Toxicity: No reproductive toxicity effects have been described for Methane.

*A mutagen is a chemical which causes permanent changes to genetic material (DNA) such that the changes will propagate through generation lines. An embryotoxin is a chemical which causes damage to a developing embryo (i.e. within the first eight weeks of pregnancy in humans), but the damage does not propagate across generational lines. A teratogen is a chemical which causes damage to a developing fetus, but the damage does not propagate across generational lines. A reproductive toxin is any substance which interferes in any way with the reproductive process.*
**BIOLOGICAL EXPOSURE INDICES (BEIs)**: Currently, Biological Exposure Indices (BEIs) have not been determined for Methane.

## 12. ECOLOGICAL INFORMATION

**ENVIRONMENTAL STABILITY**: This gas will be dissipated rapidly in well-ventilated areas.
**EFFECT OF MATERIAL ON PLANTS or ANIMALS**: Due to the small cylinder size no adverse effect on animals or animals would be anticipated if one cylinder of this product is released.
**EFFECT OF CHEMICAL ON AQUATIC LIFE**: No evidence is currently available on this product's effects on aquatic life.

## 13. DISPOSAL CONSIDERATIONS

**PREPARING WASTES FOR DISPOSAL**: Waste disposal must be in accordance with appropriate Federal, State, and local regulations. Cylinders with undesired residual product may be safely vented outdoors with the proper regulator. For further information, refer to Section 16 (Other Information).

## 14. TRANSPORTATION INFORMATION

**THIS GAS IS HAZARDOUS AS DEFINED BY 49 CFR 172.101 BY THE U.S. DEPARTMENT OF TRANSPORTATION.**

**PROPER SHIPPING NAME:** Methane, compressed
**HAZARD CLASS NUMBER and DESCRIPTION:** 2.1 (Flammable Gas)
**UN IDENTIFICATION NUMBER:** UN 1971
**PACKING GROUP:** Not applicable.
**DOT LABEL(S) REQUIRED:** Class 21. (Flammable Gas)
**NORTH AMERICAN EMERGENCY RESPONSE GUIDEBOOK NUMBER (2000):** 115
**MARINE POLLUTANT**: Methane is not classified by the DOT as Marine Pollutants (as defined by 49 CFR 172.101, Appendix B).
**SPECIAL SHIPPING INFORMATION:** Cylinders should be transported in a secure position, in a well-ventilated vehicle. The transportation of compressed gas cylinders in automobiles or in closed-body vehicles can present serious safety hazards. If transporting these cylinders in vehicles, ensure these cylinders are not exposed to extremely high temperatures (as may occur in an enclosed vehicle on a hot day). Additionally, the vehicle should be well-ventilated during transportation.
**Note:** DOT 39 Cylinders ship in a strong outer carton (overpack). Pertinent shipping information goes on the outside of the overpack. DOT 39 Cylinders do not have transportation information on the cylinder itself.

**TRANSPORT CANADA TRANSPORTATION OF DANGEROUS GOODS REGULATIONS**: This gas is considered as Dangerous Goods, per regulations of Transport Canada.

**PROPER SHIPPING NAME:** Methane, compressed
**HAZARD CLASS NUMBER and DESCRIPTION:** 2.1 (Flammable Gas)
**UN IDENTIFICATION NUMBER:** UN 1971
**PACKING GROUP:** Not Applicable
**HAZARD LABEL:** Class 2.1 (Flammable Gas)
**SPECIAL PROVISIONS:** None
**EXPLOSIVE LIMIT AND LIMITED QUANTITY INDEX:** 0.12
**ERAP INDEX:** 3000
**PASSENGER CARRYING SHIP INDEX:** Forbidden
**PASSENGER CARRYING ROAD VEHICLE OR PASSENGER CARRYING RAILWAY VEHICLE INDEX:** Forbidden
**NORTH AMERICAN EMERGENCY RESPONSE GUIDEBOOK NUMBER (2000):** 115

## 15. REGULATORY INFORMATION

**NOTE:** Shipment of compressed gas cylinders via Public Passenger Road Vehicle is a violation of Canadian law (Transport Canada Transportation of Dangerous Goods Act, 1992).

**ADDITIONAL U.S. REGULATIONS:**

**U.S. SARA REPORTING REQUIREMENTS**: This gas is not subject to the reporting requirements of Sections 302, 304 and 313 of Title III of the Superfund Amendments and Reauthorization Act., as follows:

**U.S. SARA THRESHOLD PLANNING QUANTITY:** There are no specific Threshold Planning Quantities for this gas. The default Federal MSDS submission and inventory requirement filing threshold of 10,000 lb (4,540 kg) may apply, per 40 CFR 370.20.
**U.S. TSCA INVENTORY STATUS**: Methane is listed on the TSCA Inventory.
**U.S. CERCLA REPORTABLE QUANTITIES (RQ)**: Not applicable.
**U.S. STATE REGULATORY INFORMATION**: Methane is covered under specific State regulations, as denoted below:

**Alaska - Designated Toxic and Hazardous Substances: Methane.**
**California - Permissible Exposure Limits for Chemical Contaminants: Methane.**
**Florida - Substance List: No.**
**Illinois - Toxic Substance List: Methane.**
**Kansas - Section 302/313 List: No.**
**Massachusetts - Substance List: Methane.**
**Michigan - Critical Materials Register:** No.
**Minnesota - List of Hazardous Substances: Methane.**
**Missouri - Employer Information/Toxic Substance List: Methane.**
**New Jersey - Right to Know Hazardous Substance List: Methane.**
**North Dakota - List of Hazardous Chemicals, Reportable Quantities: No.**
**Pennsylvania - Hazardous Substance List: Methane.**
**Rhode Island - Hazardous Substance List: Methane.**
**Texas - Hazardous Substance List: No.**
**West Virginia - Hazardous Substance List: No.**
**Wisconsin - Toxic and Hazardous Substances: No.**

**CALIFORNIA SAFE DRINKING WATER AND TOXIC ENFORCEMENT ACT (PROPOSITION 65):** Methane is not on the California Proposition 65 lists.

**OTHER U.S. FEDERAL REGULATIONS**:
- Methane does not contain any Class I or Class II ozone depleting chemicals (40 CFR part 82).
- Methane is subject to the reporting requirements of Section 112(r) of the Clean Air Act. The Threshold Quantity for of this gas is 10,000 pounds.
- Depending on specific operations involving the use of this product, the regulations of the Process Safety Management of Highly Hazardous Chemicals may be applicable (29 CFR 1910.119). Under this regulation Methane is not listed in Appendix A, however, any process that involves a flammable gas on-site, in one location, in quantities of 10,000 lbs (4,553 kg) or greater is covered under this regulation unless it is used as a fuel.
- Methane is listed as a Regulated Substance, per 40 CFR, Part 68, of the Risk Management for Chemical Releases as a flammable substance.

**ADDITIONAL CANADIAN REGULATIONS:**

**CANADIAN DSL/NDSL INVENTORY STATUS:** Methane on the Canadian DSL Inventory.

**CANADIAN ENVIRONMENTAL PROTECTION ACT (CEPA) PRIORITIES SUBSTANCES LISTS:** Methane is not on the CEPA Priorities Substances List.

**CANADIAN WHMIS CLASSIFICATION:** Methane is categorized as a Controlled Product, Hazard Classes A and B1, as per the Controlled Product Regulations.

## 16. OTHER INFORMATION

### INFORMATION ABOUT DOT-39 NRC (Non-Refillable Cylinder) PRODUCTS

DOT 39 cylinders ship as hazardous materials when full. Once the cylinders are relieved of pressure (empty) they are not considered hazardous material or waste. Residual gas in this type of cylinder is not an issue because toxic gas mixtures are prohibited. Calibration gas mixtures typically packaged in these cylinders are Nonflammable n.o.s., UN 1956. A small percentage of calibration gases packaged in DOT 39 cylinders are flammable gas mixtures.

For disposal of used DOT-39 cylinders, it is acceptable to place them in a landfill if local laws permit. Their disposal is no different than that employed with other DOT containers such as spray paint cans, household aerosols, or disposable cylinders of propane (for camping, torch etc.). When feasible, we recommended recycling for scrap metal content. CALGAZ will do this for any customer that wishes to return cylinders to us prepaid. All that is required is a phone call to make arrangements so we may anticipate arrival. Scrapping cylinders involves some preparation before the metal dealer may accept them. We perform this operation as a service to valued customers who want to participate.

**MIXTURES:** When two or more gases or liquefied gases are mixed, their hazardous properties may combine to create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an Industrial Hygienist or other trained person when you make your safety evaluation of the end product. Remember, gases and liquids have properties which can cause serious injury or death.

Further information can be found in the following pamphlets published by: Compressed Gas Association Inc. (CGA), 1725 Jefferson Davis Highway, Suite 1004, Arlington, VA 22202-4102. Telephone: (703) 412-0900.

| | |
|---|---|
| *P-1* | *"Safe Handling of Compressed Gases in Containers"* |
| *P-14* | *"Accident Prevention in Oxygen-Rich and Oxygen Deficient Atmospheres"* |
| *SB-8* | *"Use of Oxy-fuel Gas Welding and Cutting Apparatus"* |
| *SB-2* | *"Oxygen Deficient Atmospheres"* |
| | *"Handbook of Compressed Gases"* |

**PREPARED BY:**
CHEMICAL SAFETY ASSOCIATES, Inc.
PO Box 3519, La Mesa, CA 91944-3519
619/670-0609

AIR LIQUIDE

AB **MATERIAL SAFETY DATA SHEET (MSDS)**

**NITROGEN**

DATE: April 2013 Version 2 Page 1 of 2

Ref. No.: MS095

**1 PRODUCT AND COMPANY IDENTIFICATION**

| | |
|---|---|
| **Product Name** | Nitrogen |
| **Chemical Formula** | $N_2$ |
| **Trade Names** | Nitrogen, Compressed (Tec)<br>Nitrogen, Instrument Grade<br>Nitrogen, Pharmaceutical Grade<br>Nitrogen, ELCAP |
| **Colour coding** | Compressed, Instrument, ultra high purity & Pharmaceutical Grades have French Grey (H.30) bodies with black shoulders. Relevant decals/stencilling shall be on bodies of cylinders. ELCAP shall have a Protea Pink (A.58) body, with "ELCAP" stencilled on body of the cylinder. |
| **Valve** | ELCAP No. 2 type-Brass 5/8inch BSP right hand female. All the other grades shall be fitted with 3 SN – Brass, ¾ inch BSP right hand female valves. |
| **Company Identification** | African Oxygen Limited<br>23 Webber Street<br>Johannesburg, 2001<br>Tel No: (011) 490-0400<br>Fax No: (011) 490-0506 |
| **EMERGENCY NUMBER** | **0860 020202 or (011) 873 4382 (24 hours)** |

**2 COMPOSITION/INFORMATION ON INGREDIENTS**

| | |
|---|---|
| Chemical Name | Nitrogen |
| Chemical Family | Inert gas |
| CAS No. | 7727-37-9 |
| UN No. | 1066 |
| ERG No. | 121 |
| Hazchem Warning | 2 C Non-flammable Gas |

**3 HAZARDS IDENTIFICATION**

**Main Hazards**
All cylinders are portable gas containers, and must be regarded as pressure vessels at all times. Nitrogen does not support life. It can act as a simple asphyxiant by diluting the concentration of oxygen in air below the levels necessary to support life.

**Adverse Health Effects**
Inhalation of nitrogen in excessive concentrations can result in dizziness, nausea, vomiting, loss of consciousness and death.

**Chemical Hazards**
Nitrogen is relatively inert to most materials under ordinary conditions. It becomes more reactive at elevated temperatures, and combines with hydrogen, oxygen and some metals.

**Biological Hazards** No known effect.

**Vapour Inhalation**
As nitrogen acts as a simple asphyxiant death may result from errors in judgement, confusion, or loss of consciousness which prevents self-rescue. At low oxygen concentrations, unconsciousness and death may occur in seconds without warning.

**4 FIRST AID MEASURES**

**Eye/Skin Contact** No known effect.
**Ingestion** (See Section 3 above)
**Inhalation**
Prompt medical attention is mandatory in all cases of overexposure to Nitrogen. Rescue personnel should be equipped with self-contained breathing apparatus. Conscious persons should be assisted to an uncontaminated area and inhale fresh air. Quick removal from the contaminated area is most important. Unconscious persons should be removed to an uncontaminated area, and given mouth-to-mouth resuscitation and supplemental oxygen.

**5 FIRE FIGHTING MEASURES**

**Extinguishing Media**
As Nitrogen is an inert gas, it does not contribute to a fire, but could help with the extinguishing by reducing the oxygen content of the air by dilution to below the level to support combustion.

**Specific Hazards**
Nitrogen does not support life. It can act as a simple asphyxiant by diluting the concentration of oxygen in the air below the levels to support life.

**Emergency Actions**
If possible, shut off the source of excess Nitrogen. Evacuate area. All cylinders should be removed from the vicinity of the fire. Cylinders that cannot be removed should be cooled with water from a safe distance. Cylinders which have been exposed to excessive heat should be clearly identified and returned to supplier. CONTACT THE NEAREST AFROX BRANCH.

**Protective Clothing**
Self-contained breathing apparatus. Safety gloves and shoes, or boots, should be worn when handling cylinders.

**Environmental Precautions**
Nitrogen is lighter than air and disperses rapidly in the atmosphere. Care should be taken when entering a potentially oxygen-deficient environment. If possible, ventilate the affected area.

**6 ACCIDENTAL RELEASE MEASURES**

**Personal Precautions**
Do not enter any area where nitrogen has been spilled unless tests have shown that it is safe to do so.

**Environmental Precautions**
Nitrogen does not pose a hazard to the environment.

**Small Spills**
Shut off the source of escaping nitrogen. Ventilate the area.

**Large Spills**
Evacuate the area. Shut off the source of the spill if this can be done without risk. Restrict access to the area until completion of the clean-up procedure. Ventilate the area using forced-draught if necessary.

**7 HANDLING AND STORAGE**

Do not allow cylinders to slide or come into contact with sharp edges. Nitrogen cylinders may be stacked horizontally provided that they are firmly secured at each end to prevent rolling. Use a "first in - first out" inventory system to prevent full cylinders from being stored for excessive periods of time. Keep out of reach of children.

**8 EXPOSURE CONTROLS/PERSONAL PROTECTION**

**Occupational Exposure Hazards**
As nitrogen is a simple asphyxiant, avoid any areas where spillage has taken place. Only enter once testing has proved the atmosphere to be safe.

**Engineering Control Measures**
Engineering control measures are preferred to reduce exposure to Oxygen-depleted atmospheres. General methods include forced-draught ventilation, separate from other exhaust ventilation systems. Ensure that sufficient fresh air enters at, or near floor level.

**Personal Protection**
Self-contained breathing apparatus should always be worn when entering area where oxygen depletion may have occurred. Safety goggles, gloves and shoes or boots should be worn when handling cylinders.

**Skin** No known effect.

**9 PHYSICAL AND CHEMICAL PROPERTIES**

**PHYSICAL DATA**

| | |
|---|---|
| Chemical Symbol | $N_2$ |
| Molecular Weight | 28,013 |
| Specific Volume @ 20°C & 101,325 kPa | 861,5ml/g |
| Density, gas @ 101,325 kPa and 20°C | 1,25 kg/m$^3$ |
| Relative density (Air = 1) @ 101,325 kPa | 0,967 |
| Colour | None |
| Taste | None |

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AB **MATERIAL SAFETY DATA SHEET (MSDS)**

**NITROGEN**

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Odour None

**10 STABILITY AND REACTIVITY**

**Conditions to avoid**
The dilution of the oxygen concentration in the atmosphere to levels which cannot support life. Never use cylinders as rollers or supports, or for any other purpose than the storage of Nitrogen. Never expose cylinders to excessive heat, as this may cause sufficient build-up of pressure to rupture the cylinders.

**Incompatible Materials**
As Nitrogen is inert it may be contained in systems constructed of any of the common metals which have been designed to safely withstand the pressures involved.

**Hazardous Decomposition Products**
None

**11 TOXICOLOGICAL INFORMATION**

| | |
|---|---|
| Acute Toxicity | No known effect |
| Skin & eye contact | No known effect |
| Chronic Toxicity | No known effect |
| Carcinogenicity | No known effect |
| Mutagenicity | No known effect |
| Reproductive Hazards | No known effect |

**(For further information see Section 3. Adverse Health effects)**

**12 ECOLOGICAL INFORMATION**

Nitrogen is lighter than air and can cause pockets of oxygen depleted atmosphere in low-lying areas. It does not pose a hazard to the ecology.

**13 DISPOSAL CONSIDERATIONS**

**Disposal Methods**
Small amounts may be blown to the atmosphere under controlled conditions. Large amounts should only be handled by the gas supplier.

**Disposal of Packaging**
The disposal of cylinders must only be handled by the gas supplier.

**14 TRANSPORT INFORMATION**

**ROAD TRANSPORTATION**

| | |
|---|---|
| UN No | 1066 |
| ERG No | 121 |
| Hazchem warning | 2C Non-flammable Gas |

**SEA TRANSPORTATION**

| | |
|---|---|
| IMDG | 1066 |
| Class | |
| Packaging group | |
| label | Non-flammable gas |

**AIR TRANSPORTATION**

| | |
|---|---|
| ICAO/IATA Code | 1066 |
| Class | 2.2 |
| Packaging group | |
| Packaging instructions | |
| - Cargo | 200 |
| - Passenger | 200 |
| Maximum quantity allowed | |
| - Cargo | 150kg |
| - Passenger | 75kg |

**15 REGULATORY INFORMATION**

EEC Hazard class Non-flammable

| Risk Phrase | Description | Safety Phrase | Description |
|---|---|---|---|
| R20 | Harmful by inhalation | S2 | Keep out of reach of Children |
| R44 | Risk of explosion if heated under confinement | S9 | Keep container in a well-ventilated place |
| | | S15 | Keep way from heat |
| | | S37 | Wear suitable gloves |
| | | S38 | In case of insufficient ventilation, wear suitable respiratory equipment |
| | | S51 | Use only in well-ventilated areas |

National legislation None

Refer to SABS 0265 for explanation of the above.

**16 OTHER INFORMATION**

**Bibliography**

Compressed Gas Association, Arlington, Virginia
Handbook of Compressed Gases – 3rd Edition
Matheson. Matheson Gas Data Book – 6th Edition
SABS 0265 - Labelling of Dangerous Substances

**17 EXCLUSION OF LIABILITY**

Information contained in this publication is accurate at the date of publication. The company does not accept liability arising from the use of this information, or the use, application, adaptation or process of any products described herein.

# MATERIAL SAFETY DATA SHEET

## SECTION 1. PRODUCT IDENTIFICATION

**PRODUCT NAME:** **Oxygen, Compressed**

**CHEMICAL NAME:** **Oxygen** **FORMULA:** $O_2$

**SYNONYMS:** Oxygen gas, Gaseous Oxygen, GOX

**MANUFACTURER:** **Air Products and Chemicals, Inc.**
7201 Hamilton Boulevard

Allentown, PA 18195 - 1501

**PRODUCT INFORMATION:** 1-800-752-1597

**MSDS NUMBER:** 1012 **REVISION:** 5

**REVISION DATE:** January 1995 **REVIEW DATE:** August 1997**

## SECTION 2. COMPOSITION / INFORMATION ON INGREDIENTS

Oxygen is sold as pure product > 99%.

**CAS NUMBER:** 7782-44-7

**EXPOSURE LIMITS:**

**OSHA:** Not established **ACGIH:** Not established **NIOSH:** Not established

## SECTION 3. HAZARD IDENTIFICATION

### EMERGENCY OVERVIEW

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

**EMERGENCY TELEPHONE NUMBERS**

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

**POTENTIAL HEALTH EFFECTS INFORMATION:**

**INHALATION:** Breathing 80% or more oxygen at atmospheric pressure for more than a few hours may cause nasal stuffiness, cough, sore throat, chest pain and breathing difficulty. Breathing oxygen at higher pressure increases the likelihood of adverse effects within a shorter time period. Breathing pure oxygen under pressure may cause lung damage and also central nervous system effects resulting in dizziness, poor coordination, tingling sensation, visual and hearing disturbances, muscular twitching, unconsciousness and convulsions. Breathing oxygen under pressure may cause prolongation of adaptation to darkness and reduced peripheral vision.

**EYE / SKIN CONTACT:** No adverse effect.

**EXPOSURE INFORMATION:**

**ROUTE OF ENTRY:**

Inhalation

**TARGET ORGANS:** Eyes, central nervous system

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

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

## SECTION 4. FIRST AID

**INHALATION:** Move victim to fresh air or if in elevated pressures reduce oxygen pressures to one atmosphere. Call a physician. The physician should be advised that the victim has been

exposed to a high concentration of oxygen. No treatment is required in the absence of symptoms or high pressure exposure.

**EYE / SKIN CONTACT:** Not applicable

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

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

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

## SECTION 5. FIRE AND EXPLOSION

| FLASH POINT: | AUTOIGNITION: | FLAMMABLE LIMITS: |
|---|---|---|
| Not applicable | Nonflammable | Nonflammable |

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

**HAZARDOUS COMBUSTION PRODUCTS:** None

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

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

## SECTION 6. ACCIDENTAL RELEASE MEASURES

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

## SECTION 7. STORAGE AND HANDLING

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

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

All gauges, valves, regulators, piping and equipment to be used in oxygen service must be cleaned for oxygen service in accordance with Compressed Gas Association pamphlet G-4.1.

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

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

**SPECIAL REQUIREMENTS:** Always store and handle compressed gases in accordance with Compressed Gas Association, Inc. (ph. 703-412-0900) pamphlet CGA P-1, *Safe Handling of*

*Compressed Gases in Containers.* Local regulations may require specific equipment for storage or use.

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

## SECTION 8. PERSONAL PROTECTION / EXPOSURE CONTROL

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

**RESPIRATORY PROTECTION:**

GENERAL USE: None required

EMERGENCY: Use SCBA do to possibility of fire when concentrations exceed 23%.

**OTHER PROTECTIVE EQUIPMENT:** Safety shoes and work gloves are recommended when handling cylinders. Clothing exposed to high concentrations may retain oxygen 30 minutes or longer and become a potential fire hazard. Stay away from ignition sources.

## ECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

**APPEARANCE:** Colorless gas

**ODOR:** Odorless

**MOLECULAR WEIGHT:** 32.0

**BOILING POINT (1 atm):** -297.3 °F (-183.0 °C)

**SPECIFIC GRAVITY (Air =1):** 1.10

**SPECIFIC VOLUME (at 70 °F 21.1 °C) and 1 atm):** 12.08 $ft^3$/lb (0.754 $m^3$/kg)

**FREEZING / MELTING POINT:** -361.9 °F (-218.8 °C)

**VAPOR PRESSURE:** Not applicable at 70°F

**GAS DENSITY (At 70°F (21.1°C) and 1 Atm):** 0.083 lb /$ft^3$ (1.326 kg/$m^3$)

**SOLUBILITY IN WATER (Vol./Vol. at 32°F (0°C)):** 0.049

## SECTION 10. REACTIVITY / STABILITY

**CHEMICAL STABILITY:** Stable

**CONDITIONS TO AVOID:** None

**INCOMPATIBILITY:** Oils, grease, hydrocarbons and flammable materials.

**HAZARDOUS DECOMPOSITION PRODUCTS:** None

**HAZARDOUS POLYMERIZATION:** Will not occur

## SECTION 11. TOXICOLOGICAL INFORMATION

At atmospheric concentration and pressure, oxygen poses no toxicity hazards.

Premature infants exposed to high oxygen concentrations may suffer delayed retinal damage which can progress to retinal detachment and blindness. Retinal damage may also occur in adults exposed to 100% oxygen for extended periods (24 to 48 hr).

At two or more atmospheres central nervous system (CNS) toxicity occurs. Symptoms include nausea, vomiting, dizziness or vertigo, muscle twitching, vision changes, and loss of consciousness and generalized seizures. At three atmospheres, CNS toxicity occurs in less than two hours, and at six atmospheres in only a few minutes.

## SECTION 12. ECOLOGICAL INFORMATION

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

## SECTION 13. DISPOSAL

**UNUSED PRODUCT / EMPTY CONTAINER:** Return container and unused product to supplier. Do not attempt to dispose of residual or unused quantities.

**DISPOSAL:** For emergency disposal, secure cylinder and slowly discharge gas to the atmosphere in a well ventilated area or outdoors.

## SECTION 14. TRANSPORTATION

**DOT HAZARD CLASS:** 2.2 (Nonflammable Gas)

**DOT SHIPPING LABEL:** Nonflammable Gas, Oxidizer

**DOT SHIPPING NAME:** Oxygen, compressed

**IDENTIFICATION NUMBER:** UN 1072

**REPORTABLE QUANTITY (RQ):** None

**PLACARD:** Nonflammable Gas or Oxygen

**SPECIAL SHIPPING INFORMATION:** Cylinders should be transported in a secure upright position in a well ventilated truck. Never transport in passenger compartment of a vehicle. An oxygen label may be used for domestic shipment in the United States and Canada in place of the Non-flammable and Oxidizer labels (49CFR Part 172).

## SECTION 15. REGULATORY INFORMATION

**U.S. FEDERAL REGULATIONS:**

**EPA - ENVIRONMENTAL PROTECTION AGENCY:**

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

CERCLA Reportable Quantity: None

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

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

Oxygen is not listed as an Extremely Hazardous Substance.

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

IMMEDIATE: No
DELAYED: No

PRESSURE: Yes
REACTIVITY: No
FIRE: Yes

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

Oxygen is not listed as a toxic chemical.

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

Oxygen is not listed as a regulated substance.

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

**OSHA - OCCUPATIONAL SAFETY AND HEALTH ADMINISTRATION**

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

Oxygen is not listed as a Highly Hazardous Chemical.

**STATE REGULATIONS**

CALIFORNIA:

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

SCAQMD Rule: VOC = Not applicable

**Material**

**Safety**

**Data**

| | |
|---|---|
| Health | 2 |
| Fire | 3 |
| Reactivity | 0 |
| Personal Protection | H |

# Sheet

# o-Xylene MSDS

## Section 1: Chemical Product and Company Identification

**Product Name:** o-Xylene

**Catalog Codes:** SLX1012

**CAS#:** 95-47-6

**RTECS:** ZE2450000

**TSCA:** TSCA 8(b) inventory: o-Xylene

**CI#:** Not applicable.

**Synonym:** 1,2-Dimethylbenzene

**Chemical Name:** o-Xylene

**Chemical Formula:** C6H4(CH3)2

**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 |
|---|---|---|
| {o-}Xylene | 95-47-6 | 100 |

**Toxicological Data on Ingredients:** o-Xylene LD50: Not available. LC50: Not available.

## Section 3: Hazards Identification

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

**Potential Chronic Health Effects:**

CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. The substance may be toxic to kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

## Section 4: First Aid Measures

Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Get medical attention.

**Skin Contact:**

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

**Serious Skin Contact:**

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

**Inhalation:**

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

**Serious Inhalation:**

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

**Ingestion:**

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

**Serious Ingestion:** Not available.

## Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 463°C (865.4°F)

**Flash Points:** CLOSED CUP: 17°C (62.6°F).

**Flammable Limits:** LOWER: 0.9% UPPER: 6.7%

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

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

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

Risks of explosion of the product in presence of mechanical impact: Not available. Slightly explosive in presence of open flames and sparks, of heat.

**Fire Fighting Media and Instructions:**

Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog.

**Special Remarks on Fire Hazards:**

Vapors are heavier than air and may travel considerable distance to source of ignition and flash back.
When heated to decomposition it emits acrid smoke and irritating fumes.

**Special Remarks on Explosion Hazards:**

Explosive in the form of vapor when exposed to heat or flame. Vapors may form explosive mixtures with air. Containers may explode when heated. Runoff to sewer may create fire or explosion hazard

## Section 6: Accidental Release Measures

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**

Toxic flammable liquid, insoluble or very slightly soluble in water. 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. 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 away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

**Storage:**

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

## Section 8: Exposure Controls/Personal Protection

**Engineering Controls:**

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

**Personal Protection:**

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

**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: 434 STEL: 651 (mg/m3) from ACGIH (TLV) [United States] TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) [United States] STEL: 150 (ppm) from NIOSH STEL: 655 (mg/m3) from NIOSHConsult local authorities for acceptable exposure limits.

## Section 9: Physical and Chemical Properties

**Physical state and appearance:** Liquid. (Mobile, nonpolar liquid.)

**Odor:** Aromatic. Sweetish.

**Taste:** Not available.

**Molecular Weight:** 106.17 g/mole

**Color:** Colorless.

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

**Boiling Point:** 144.4°C (291.9°F)

**Melting Point:** -25°C (-13°F)

**Critical Temperature:** 359°C (678.2°F)

**Specific Gravity:** 0.88 (Water = 1)

**Vapor Pressure:** 0.9 kPa (@ 20°C)

**Vapor Density:** 3.7 (Air = 1)

**Volatility:** Not available.

**Odor Threshold:** 0.05 ppm

**Water/Oil Dist. Coeff.:** The product is more soluble in oil; log(oil/water) = 3.1

**Ionicity (in Water):** Not available.

**Dispersion Properties:**

Dispersed in diethyl ether. Is not dispersed in cold water, hot water. See solubility in diethyl ether, acetone.

**Solubility:**

Soluble in diethyl ether, acetone. Insoluble in cold water, hot water.

## Section 10: Stability and Reactivity Data

**Stability:** The product is stable.

**Instability Temperature:** Not available.

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

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

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

**Special Remarks on Reactivity:**

Photochemically reactive. Incompatible with strong oxidizers(e.g. chlorine, bromine, fluorine), and strong acids (e.g. nitric acid, acetic acid).

**Special Remarks on Corrosivity:** Not available.

**Polymerization:** Will not occur.

## Section 11: Toxicological Information

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

**Toxicity to Animals:**

Lowest Published Lethal Dose - Inhalation (LCL): 6125 ppm 12 hours [Rat]; 6125 ppm 12 hours [Human]
Lowest Published Lethal Dose - Oral: 5000 mg/kg [Rat]

**Chronic Effects on Humans:**

CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/ toxin/male [POSSIBLE]. May cause damage to the following organs: kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

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

**Special Remarks on Toxicity to Animals:** Not available.

**Special Remarks on Chronic Effects on Humans:**

May cause adverse reproductive effects (male) and birth defects based on animal data. 0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

**Special Remarks on other Toxic Effects on Humans:**

Acute Potential Health Efffects Skin: May cause skin irritation. May be absorbed through skin i harmful amounts. Eyes: Causes severe eye irritation. Inhalation: Causes respiratory tract and mucous membranes irritation. May affect sense organs, behavior (Central Nervous system) which may result in dizziness, general weakness, central nervous system depression, confusion, ataxia, disorientation, lethargy, drowsiness, headaches. May also affect respiration, cardiovascular system, liver, blood, and digestive system (nausea, vomiting) Ingestion: Harmful if swallowed. Causes digestive tract irritation with nausea, vomiting and diarrhea. May also affect metabolism, liver, and urinary system, and central nervous system (excitement followed by headache, dizziness, drowsiness and nausea). Chronic Potential Health Effects: Skin: Prolonged or repeated contact may cause defatting of skin and dermatitis. Eyes: Prolonged or repeated exposure may cause conjunctivitis or permanent eye damage. Inhalation: Chronic inhalation may cause effects similar to those of acute inhalation.

## Section 12: Ecological Information

**Ecotoxicity:** Not available.

**BOD5 and COD:** Not available.

**Products of Biodegradation:**

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

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

**Special Remarks on the Products of Biodegradation:** Not available.

## Section 13: Disposal Considerations

**Waste Disposal:**

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

## Section 14: Transport Information

**DOT Classification:** CLASS 3: Flammable liquid.

**Identification:** : Xylene UNNA: 1307 PG: III

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

## Section 15: Other Regulatory Information

**Federal and State Regulations:**

Connecticut hazardous material survey.: o-Xylene Illinois chemical safety act: o-Xylene New York release reporting list: o-Xylene Pennsylvania RTK: o-Xylene Florida: o-Xylene Massachusetts RTK: o-Xylene Massachusetts spill list: o-Xylene New Jersey: o-Xylene New Jersey spill list: o-Xylene Louisiana spill reporting: o-Xylene California Director's List of Hazardous Substances: o-Xylene TSCA 8(b) inventory: o-Xylene TSCA 8(d) H and S data reporting: o-Xylene: Effective: 10/4/82; Sunset: 10/4/92 SARA 313 toxic chemical notification and release reporting: o-Xylene CERCLA: Hazardous substances.: o-Xylene: 1000 lbs. (453.6 kg)

**Other Regulations:**

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

**Other Classifications:**

**WHMIS (Canada):**

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

**DSCL (EEC):**

**HMIS (U.S.A.):**

**Health Hazard:** 2

**Fire Hazard:** 3

**Reactivity:** 0

**Personal Protection:** h

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

**Health:** 2

**Flammability:** 3

**Reactivity:** 0

**Specific hazard:**

**Protective Equipment:**

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

## Section 16: Other Information

**References:**

-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

**Other Special Considerations:** Not available.

**Created:** 10/11/2005 12:54 PM

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

# MATERIAL SAFETY DATA SHEET FOR ODORIZED PROPANE

## 1. Chemical Product and Company Identification

**Product Name:** Odorized Commercial Propane
**Chemical Name:** Propane
**Chemical Family:** Paraffinic Hydrocarbon
**Formula:** $C_3H_8$
**Synonyms**: Dimethylmethane, LP-Gas, Liquefied Petroleum Gas (LPG), Propane, Propyl Hydride

**Transportation Emergency Number:**
**CHEMTREC 1-800-424-9300**

**Name & Address:**
**AmeriGas Propane, L.P.**
**P. O. Box 965**
**Valley Forge, PA. 19482**

**For General Information, Call:**
**1-610-337-1000, Safety Dept.**

## 2. Composition / Information on Ingredients

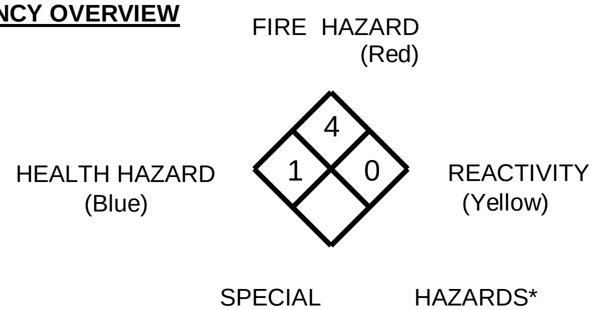
| INGREDIENT NAME /CAS NUMBER | PERCENTAGE | OSHA PEL | ACGIH TLV |
|---|---|---|---|
| Propane / 74-98-6 | 87.5 -100 | | Simple asphyxiant |
| Ethane / 74-84-0 | 0 - 7.0 | | Simple asphyxiant |
| Propylene / 115-07-1 | 0 - 5.0 | 1,000 ppm | Simple asphyxiant |
| Butanes / 106-97-8 | 0 - 2.5 | | Simple asphyxiant |
| Ethyl Mercaptan / 75-08-1 | 0 - 50 ppm | | 0.5 ppm |
| | | 0.5 ppm | |

**WARNING:** The intensity of the chemical odorant (e.g., ethyl mercaptan) may "fade" or diminish due to chemical oxidation, adsorption or absorption. Individuals with nasal perception problems may not be able to smell the odorant. Leaking propane from underground gas lines may lose its odor as it passes through certain soils. No odorant is effective 100% of the time. Therefore, circumstances can exist when individuals are in the presence of leaking propane and not be alerted by the smell. Contact AmeriGas for more information about odor, propane gas detectors and other safety considerations associated with the handling, storage and use of propane.

## 3. Hazards Identification

**EMERGENCY OVERVIEW**

**DANGER!** Flammable liquefied gas under pressure. Keep away from heat, sparks, flame, and all other ignition sources. Vapor replaces oxygen available for breathing and may cause suffocation in confined spaces. Use only with adequate ventilation. Reliance upon detection of odor may not provide adequate warning of potentially hazardous concentrations. Vapor is heavier than air; may collect at low levels. Liquid can cause freeze burn similar to frostbite. Do not get liquid in eyes, on skin, or on clothing. Avoid breathing vapor. Keep service valve closed when not in use.




Minimal 0 Slight 1 Moderate 2 Serious 3 Severe 4
*(Ref. NFPA 704)

**POTENTIAL HEALTH EFFECTS INFORMATION**

**ROUTES OF EXPOSURE:**

**Inhalation:** Asphyxiation. Before suffocation could occur, the lower flammability limit of propane in air would be exceeded, possibly causing both an oxygen-deficient and explosive atmosphere. Exposure to concentrations >10% may cause dizziness. Exposure to atmospheres containing 19% or less oxygen will bring about unconsciousness without warning. Lack of sufficient oxygen may cause serious injury or death.
**Eye Contact:** Contact with liquid can cause freezing of tissue.
**Skin Contact:** Contact with liquid can cause frostbite.
**Skin Absorption:** None.

**Ingestion:** Ingestion is not expected to occur in normal use. However, liquid can cause freeze burn similar to frostbite.

**CHRONIC EFFECTS:** None. **CARCINOGENICITY:** Propane is not listed by NTP, OSHA or IARC.

## 4. First Aid Measures

**INHALATION:** Individuals suffering from lack of oxygen should be removed to fresh air. If victim is not breathing, administer artificial respiration. If breathing is difficult, administer oxygen. Obtain immediate medical assistance.

**EYE CONTACT:** Gently flush eyes with lukewarm water. Obtain immediate medical assistance.

**SKIN CONTACT:** Remove saturated clothes, shoes and jewelry. Immerse affected area in lukewarm water not exceeding 105° F. Keep immersed. Obtain immediate medical assistance.

1

**INGESTION:** If swallowed, obtain immediate medical assistance.

## 5. Fire Fighting Measures

**IGNITION TEMPERATURE IN AIR:** 920°F to 1120°F (493°C to 549°C) **FLAMMABLE LIMITS IN AIR (% by volume):** Lower: 2.15% Upper: 9.6%

**EXTINGUISHING MEDIA:** Dry chemical, $CO_2$, water spray or fog for surrounding area. Do not attempt to extinguish fire until propane source is isolated.

**SPECIAL FIRE-FIGHTING INSTRUCTIONS:** Evacuate all unnecessary personnel from the area. Allow only properly trained and protected emergency response personnel in area. A NIOSH approved self-contained breathing apparatus may be required. If gas flow cannot be shut off, do not attempt to extinguish fire. Allow fire to burn itself out. Use high volume water supply to cool exposed pressure containers and nearby equipment. Approach a flame-enveloped container from the sides, never from the ends. Use extreme caution when applying water to a container that has been exposed to heat or flame for more than a short time. For uncontrollable fires and/or when flame is impinging on container, withdraw all personnel and evacuate vicinity immediately.

**UNUSUAL FIRE AND EXPLOSION HAZARDS:** Propane is heavier than air and can collect in low areas. Flash back along a vapor trail is possible. Pressure in a container can build up due to heat; and, container may rupture suddenly and violently without warning if pressure relief devices fail to function properly. If flames are against the container, withdraw immediately on hearing a rising sound, if venting increases in volume or intensity or if there is discoloration of the container due to fire. Propane released from a properly functioning relief valve on an overheated container can also become ignited.

**HAZARDOUS COMBUSTION PRODUCTS:** None.

## 6. Accidental Release Measures

**IF MATERIAL IS RELEASED OR SPILLED:** Evacuate the immediate area. Eliminate any possible sources of ignition and provide maximum ventilation. Shut off source of propane, if possible. If leaking from container or valve, contact your supplier or AmeriGas immediately.

## 7. Handling and Storage

**HANDLING PRECAUTIONS:** Propane vapor is heavier than air and can collect in low areas that are without sufficient ventilation. Conduct system checks for leaks with a leak detector or solution, never with flame. Make certain the container service valve is shut off prior to connecting or disconnecting. If container valve does not operate properly, discontinue use and contact AmeriGas. Never insert an object (e.g., wrench, screwdriver, pry bar, etc.) into pressure relief valve or cylinder valve cap openings. Do not drop or abuse cylinders. Never strike an arc on a gas container or make a container part of an electrical circuit. See Section 16, "OTHER INFORMATION", for additional precautions.

**STORAGE PRECAUTIONS:** Store in a safe, authorized location (outside, detached storage is preferred) with adequate ventilation. Specific requirements are listed in NFPA 58, LP-GAS CODE. Isolate from heat and ignition sources. Containers should never be allowed to reach temperature exceeding 125°F (52°C). Isolate from combustible materials. Provide separate storage locations for other compressed and flammable gases. Propane containers should be separated from oxygen cylinders or other oxidizers by a minimum distance of 20 feet, or by a barrier of non-combustible material at least 5 feet high having a fire rating of at least 1/2 hour. Full and empty cylinders should be segregated. Keep cylinders in an upright position at all times so that each pressure relief valve communicates with the vapor space. Keep container valve closed and plugged or capped when not in use. Install protective caps when cylinders are not connected for use. Empty containers retain some residue and should be treated as if they were full.

## 8. Exposure Control / Personal Protection

**ENGINEERING CONTROLS**

Ventilation: Provide ventilation adequate to ensure propane does not reach a flammable mixture.

**RESPIRATORY PROTECTION**

**General Use**: None.

**Emergency Use:** If concentrations are high enough to warrant supplied-air or NIOSH self-contained breathing apparatus, then the atmosphere may be flammable (See Section 5). Appropriate precautions must be taken regarding flammability.

**PROTECTIVE CLOTHING:** Avoid skin contact with liquid propane because of possibility of freeze burn. Wear gloves and protective clothing that are impervious to the product for the duration of the anticipated exposure.

**EYE PROTECTION:** Safety glasses, goggles or face shields are recommended when handling cylinders.

## 9. Physical and Chemical Properties

**BOILING POINT:** @ 14.7 psia = -44° F (@1.00 atm.pressure = -42°C) **SPECIFIC GRAVITY OF VAPOR** (Air = 1) at 60° F (15.56°C): 1.50

**SPECIFIC GRAVITY OF LIQUID** (Water = 1) at 60° F: 0.504

**VAPOR PRESSURE**: @ 70° F (20°C) = 127 psig; @ 105° F (45°C ) = 210 psig; @ 130°F (55°C) = 287 psig

**EXPANSION RATIO** (From liquid to gas @ 14.7 psia): 1 to 270 **SOLUBILITY IN WATER:** Slight, 0.1 to 1.0%

**APPEARANCE AND ODOR:** A colorless and tasteless gas at normal temperature and pressure. An odorant (ethyl mercaptan) is added to provide a strong unpleasant odor. Should a propane-air mixture reach the lower limits of flammability, the ethyl mercaptan concentration will be approximately 0.5 ppm in air.

**ODORANT WARNING:** Odorant is added to aid in the detection of leaks. One common odorant is ethyl mercaptan, CAS No. 75-08-1. Odorant has a foul smell. The ability of people to detect odors varies widely. Also, the odor level can be reduced by certain chemical reactions with material in the propane system or when fugitive propane gas from underground leaks passes through certain soils. No odorant will be 100% effective in all circumstances. If the presence of the odorant is not obvious, notify AmeriGas immediately.

## 10. Stability and Reactivity

**STABILITY:** Stable.

**Conditions to Avoid:** Keep away from high heat, strong oxidizing agents and sources of ignition.

**REACTIVITY:**

**Hazardous Decomposition Products**: Under fire conditions, fumes, smoke, carbon monoxide, aldehydes and other decomposition products. In most applications where there is inadequate venting to the outside air, incomplete combustion will produce carbon monoxide (a toxic gas) and potentially develop concentrations that can create a serious health hazard.
**Hazardous Polymerization:** Will not occur.

## 11. Toxicological Information

Propane is non-toxic and is a simple asphyxiant. It has slight anesthetic properties. Higher concentrations may cause dizziness.

**IRRITANCY OF MATERIAL:** None. **REPRODUCTIVE EFFECTS:** None **TERATOGENICITY:** None

**SENSITIZATION TO MATERIAL:** None **MUTAGENICITY:** None **SYNERGISTIC MATERIALS:** None

## 12. Ecological Information

No adverse ecological effects are expected. Propane does not contain any Class I or Class II ozone-depleting chemicals (40 CFR Part 82). Propane is not listed as a marine pollutant by DOT (49 CFR Part 171).

## 13. Disposal Considerations

**WASTE DISPOSAL METHOD:** Do not attempt to dispose of residual or unused product in the container; return it to your supplier or contact AmeriGas for safe disposal. Residual product within a process system may be burned at a controlled rate if a suitable burning unit is available on site, and is done in accordance with federal, state and local regulations.

## 14. Transport Information

**DOT SHIPPING NAME:** Liquefied Petroleum Gas **IDENTIFICATION NUMBER:** UN 1075 **IMO SHIPPING NAME:** Propane

**IMO IDENTIFICATION NUMBER:** UN 1978 **HAZARD CLASS**: 2.1 (Flammable Gas) **PRODUCT RQ:** None

**SHIPPING LABEL (S):** Flammable Gas **PLACARD (WHEN REQUIRED):** Flammable Gas

**SPECIAL SHIPPING INFORMATION:** Container must be transported in a well-ventilated vehicle, secured, and in a position such that the pressure relief device is in communication with the vapor space.

## 15. Regulatory Information

The following information concerns U.S. Federal regulatory requirements potentially applicable to this product. Not all such requirements are identified. Users of this product are responsible for their own regulatory compliance on a federal, state [provincial] and local level.

### U.S. FEDERAL REGULATIONS

**Environmental Protection Agency (EPA)**

*Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA)* - 40 CFR Parts 117 and 302

**Reportable Quantity (RQ):** None

*Superfund Amendment and Reauthorization Act (SARA)*

- Sections 302/304: Relates to emergency planning on threshold planning quantities (TPQ) and release reporting based on reportable quantities (RQ) of EPA's extremely hazardous substances (40 CFR Part 355).

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

- Sections 311/312: Relates to submission of material safety data sheets (MSDSs) and chemical inventory reporting with identification of EPA-defined hazard classes (40 CFR Part 370). The hazard classes for this product are:
  **IMMEDIATE:** No **PRESSURE:** Yes **DELAYED:** No **REACTIVITY:** No **FLAMMABLE:** Yes

- Section 313: Relates to submission of annual reports of release of toxic chemicals that appear in 40 CFR Part 372. Propane does not require reporting under Section 313.

**Toxic Substance Control Act (TSCA)** Propane is listed on the TSCA inventory.

**Occupational Safety and Health Administration (OSHA) The following 29 CFR Parts may apply to propane:**

**29 CFR 1910.110:** *Storage and Handling of Liquefied Petroleum Gases*

**29 CFR 1910.119:** *Process Safety Management of Highly Hazardous Chemicals* **29 CFR 1910.1200:** *Hazardous Communications*

**Food and Drug Administration (FDA)**

**21 CFR 184.1655:** Generally recognized as safe (GRAS) as a direct human food ingredient when used as a propellant, aerating agent and gas.

## 16. Other Information

**SPECIAL PRECAUTIONS**: Use piping and equipment adequately designed to withstand pressure to be encountered. NFPA 58, LP-GAS CODE and OSHA 29 CFR 1910.10 require that all persons employed in handling LP-gases be trained in proper handling and operating procedures, which the employer shall document. Contact your propane supplier or AmeriGas to arrange for the required training. Allow only trained and qualified persons to install and service propane containers and systems.

**ISSUE INFORMATION**

**Issue Date: December 2002 Issued By: Director of Safety**

**Supersedes Date: April 2002 Phone Number: 1-610-337-7000**

This material safety data sheet and the information it contains is offered to you in good faith as accurate. This Supplier does not manufacture this product, but is a supplier of the product that is independently produced by others. Much of the information contained in this data sheet was received from sources outside our Company. To the best of our knowledge this information is accurate, but this Supplier does not guarantee its accuracy or completeness. Health and safety precautions in this data sheet may not be adequate for all individuals and/or situations. It is the user's obligation to evaluate and use this product safely, comply with all applicable laws and regulations and to assume the risks involved in the use of this product.

# MATERIAL SAFETY DATA SHEET (MSDS) PROPYLENE

## CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

**GAS INNOVATIONS**
**18005 E. Hwy 225**
**La Porte, TX 77571**
**Information: 281-471-2200**

**Emergency Contact:**

**3 E Company 866-303-2640**

**Calls Originating Outside the US:**

**281-471-2200 (Collect Calls Accepted)**

**SUBSTANCE: PROPYLENE**

Date prepared: September 7, 2007

| | | |
|---|---|---|
| **PRODUCT IDENTIFICATION** | ▪D.O.T. SHIPPING NAME | Propylene |
| | ▪SYNONYM (S) | Propene |
| | ▪D.O.T. I.D. NUMBER | UN-1077 |
| | ▪D.O.T. HAZZARD CLASS | 2.1 Flammable Gas |
| | ▪D.O.T. LABEL (S) | Flammable Gas |
| | ▪C.A.S. NUMBER | 115-07-01 |
| | ▪CHEMICAL FORMULA | $C_3H_6$ or $CH_3CH: CH_2$ |
| **PHYSICAL DATA** | ▪MOLECULAR WEIGHT | 42.081 |
| | ▪FREEZING POINT | -185.2°C, -301.4°F |
| | ▪BOILING POINT | -47.7°C, -53.9 °F |
| | ▪VAPOR PRESSURE | 942 kPa (gauge), 136.5 psig |
| | ▪SPECIFIC VOLUME | 0.567 $m^3$/kg, 9.06$ft_3$/lb @ 1 atm, 21.1°C |
| | ▪RELATIVE DENSITY, (air=1) | 1.48 @ 1 atm, 20°C |
| | ▪SOLUBILITY IN WATER | 22.05 $cm^3$/100 ml @ 1 atm, 20°C |
| | ▪DESCRIPTION | At room temperature and atmospheric pressure propylene is a colorless, flammable, relatively nontoxic gas, with a characteristic natural gas odor. It is shipped as a liquefied gas under its own vapor pressure. |
| **FIRE AND EXPLOSION HAZARD DATA** | ▪FLAMMABLE LIMITS IN AIR | 2.0 – 11.1 % by volume |
| | ▪AUTO-IGNITION TEMPERATURE | 480.0°C, 896.0°F |
| | ▪FIRE FIGHTING PROCEDURES | The only safe way to extinguish a propylene fire is to stop the flow of gas. IF the flow cannot be stopped, let the fire burn out while cooling the cylinder and the surroundings using a water spray. Personnel may have to wear approach-type protective suits and positive pressure self-contained breathing apparatus. Firefighters' turnout gear may be inadequate. |
| | ▪ UNUSUAL HAZARDS | 1. Cylinders exposed to fire may rupture with violent |

force. Extinguish surrounding fire and keep cylinders cool by applying water from a maximum possible distance with a water spray.

2. Flammable gases may spread from a spill after the fire is extinguished and be subject to re-ignition.

| | | |
|---|---|---|
| **HEALTH HAZARD DATA** | ▪ PERMISSIBLE EXPOSURE LIMITS | OSHA TWA None established.<br>ASGIH TWA None established. |
| | ▪ ACCUTE EFFECTS OVEREXPOSURE | Propylene is nontoxic but can act as a simple asphyxiant by displacing air. Symptoms of asphyxia include rapid respirations, dizziness and fatigue. Contact with the liquid phase or with the cold gas escaping from cylinder may cause frostbite. |
| | ▪ CHRONIC EFFECTS OF OVEREXPOSURE | None known. |
| **FIRST AID INFORMATION** | ▪ INHALATION | Move victim to fresh air. If not breathing, give artificial respiration, preferably mouth-to-mouth. If breathing is difficult, give oxygen. Call a physician. |
| | ▪ CONTACT | Treat for frostbite. |
| **REACTIVITY DATE** | ▪ STABILITY | ( X ) Stable. ( ) Unstable. |
| | ▪ INCOMPATIBILITY | Oxidizing material. |
| | ▪ HAZARDOUS DECOMPOSITION/ OXIDATION PRODUCTS | Carbon monoxide, carbon dioxide |
| | ▪ POLYMERIZATION | ( X ) Will not occur ( ) May Occur |
| **SPILL OR LEAKAGE PROCEDURE** | Shut off all ignition sources and ventilate the area. For controlling large flows, personnel may have to wear approach-type protective suits and self-contained breathing apparatus. | |
| **PRECAUTIONS** | ▪ STORAGE RECOMMENDATIONS | Cylinders should be stored and used in dry, well-ventilated areas away from sources of heat or ignition. Do not store with oxidizers. |
| | ▪ PERSONAL PROTECTIVE EQUIPMENT | 1. Eye protection – Safety glasses should be worn.<br>2. Respiratory protection – Approved respiratory equipment must bet be worn when airborne concentrations exceed safe levels.<br>3. Skin protection – No special equipment is required. Gloves are recommended for cylinder handling. |
| | ▪ BEFORE USING THE GAS | 1. Secure the cylinder to prevent it from falling or being knocked over.<br>2. Install check valves or traps to prevent suckback to the cylinder.<br>3. Ground all lines and equipment.<br>4. Leak check the lines and equipment.<br>5. Have an emergency plan covering steps to be taken in the even of an accidental release. |

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| | |
|---|---|
| Health | 2 |
| Fire | 3 |
| Reactivity | 0 |
| Personal Protection | H |

# Material Safety Data Sheet

## p-Xylene MSDS

### Section 1: Chemical Product and Company Identification

**Product Name:** p-Xylene

**Catalog Codes:** SLX1120

**CAS#:** 106-42-3

**RTECS:** ZE2625000

**TSCA:** TSCA 8(b) inventory: p-Xylene

**CI#:** Not applicable.

**Synonym:** p-Methyltoluene

**Chemical Name:** 1,4-Dimethylbenzene

**Chemical Formula:** C6H4(CH3)2

**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 |
|---|---|---|
| {p-}Xylene | 106-42-3 | 100 |

**Toxicological Data on Ingredients:** p-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 12400 mg/ kg [Rabbit.]. VAPOR (LC50): Acute: 4550 ppm 4 hour(s) [Rat].

### Section 3: Hazards Identification

**Potential Acute Health Effects:**

Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. 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 eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

## Section 4: First Aid Measures

**Eye Contact:** Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

**Skin Contact:**

After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

**Serious Skin Contact:**

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

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

**Serious Inhalation:** Not available.

**Ingestion:**

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

**Serious Ingestion:** Not available.

## Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 527°C (980.6°F)

**Flash Points:** CLOSED CUP: 25°C (77°F). OPEN CUP: 28.9°C (84°F) (Cleveland).

**Flammable Limits:** LOWER: 1.1% UPPER: 7%

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

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

**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, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use 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:**

Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

**Special Remarks on Explosion Hazards:** Not available.

## Section 6: Accidental Release Measures

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**

Toxic flammable liquid, insoluble or very slightly soluble in water. 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. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

## Section 7: Handling and Storage

**Precautions:**

Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. 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.

**Storage:**

Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

## Section 8: Exposure Controls/Personal Protection

**Engineering Controls:**

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

**Personal Protection:**

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

**Personal Protection in Case of a Large Spill:**

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

**Exposure Limits:**

TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIHConsult local authorities for acceptable exposure limits.

## Section 9: Physical and Chemical Properties

**Physical state and appearance:** Liquid. (Liquid.)

**Odor:** Not available.

**Taste:** Not available.

**Molecular Weight:** 106.17 g/mole

**Color:** Colorless.

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

**Boiling Point:** 138°C (280.4°F)

**Melting Point:** 12°C (53.6°F)

**Critical Temperature:** Not available.

**Specific Gravity:** 0.86 (Water = 1)

**Vapor Pressure:** 9 mm of Hg (@ 20°C)

**Vapor Density:** 3.7 (Air = 1)

**Volatility:** Not available.

**Odor Threshold:** 0.62 ppm

**Water/Oil Dist. Coeff.:** Not available.

**Ionicity (in Water):** Not available.

**Solubility:**

Easily soluble in methanol, diethyl ether. Insoluble in cold water, hot water.

## Section 10: Stability and Reactivity Data

**Stability:** The product is stable.

**Instability Temperature:** Not available.

**Conditions of Instability:** Not available.

**Incompatibility with various substances:** Reactive with oxidizing agents.

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

**Special Remarks on Reactivity:** Not available.

**Special Remarks on Corrosivity:** Not available.

**Polymerization:** No.

## Section 11: Toxicological Information

**Routes of Entry:** Eye contact.

**Toxicity to Animals:**

WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 5000 mg/kg [Rat.]. Acute dermal toxicity (LD50): 12400 mg/kg

[Rabbit.]. Acute toxicity of the vapor (LC50): 4550 ppm 4 hour(s) [Rat].

**Chronic Effects on Humans:** The substance is toxic to blood, kidneys, the nervous system, liver.

**Other Toxic Effects on Humans:**

Very hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation.

**Special Remarks on Toxicity to Animals:** Not available.

**Special Remarks on Chronic Effects on Humans:**

0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

**Special Remarks on other Toxic Effects on Humans:** Material is irritating to mucous membranes and upper respiratory tract.

## Section 12: Ecological Information

**Ecotoxicity:** Not available.

**BOD5 and COD:** Not available.

**Products of Biodegradation:**

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

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

**Special Remarks on the Products of Biodegradation:** Not available.

## Section 13: Disposal Considerations

**Waste Disposal:**

## Section 14: Transport Information

**DOT Classification:** Class 3: Flammable liquid.

**Identification:** : Xylene : UN1307 PG: III

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

## Section 15: Other Regulatory Information

**Federal and State Regulations:**

Pennsylvania RTK: p-Xylene Florida: p-Xylene Massachusetts RTK: p-Xylene New Jersey: p-Xylene TSCA 8(b) inventory: p-Xylene SARA 313 toxic chemical notification and release reporting: p-Xylene CERCLA: Hazardous substances.: p-Xylene

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

**Other Classifications:**

**WHMIS (Canada):**

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

**DSCL (EEC):**

R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes. R48/20- Harmful: danger of serious damage to health by prolonged exposure through inhalation.

**HMIS (U.S.A.):**

**Health Hazard:** 2

**Fire Hazard:** 3

**Reactivity:** 0

**Personal Protection:** h

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

**Health:** 2

**Flammability:** 3

**Reactivity:** 0

**Specific hazard:**

**Protective Equipment:**

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

## Section 16: Other Information

**References:**

-Hawley, G.G.. The Condensed Chemical Dictionary, 11e ed., New York N.Y., Van Nostrand Reinold, 1987. -Material safety data sheet emitted by: la Commission de la SantÃ© et de la SÃ©curitÃ© du Travail du QuÃ©bec. -SAX, N.I. Dangerous Properties of Indutrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du rÃ¨glement sur le transport des marchandises dangeureuses au canada. Centre de conformitÃ© internatinal LtÃ©e. 1986.

Toluene

**MSDS Number: M1003**
**Effective Date: 9/07/2004**

# Material Safety Data Sheet Toluene

## Section 1 - Chemical Product and Company Identification

**MSDS Name:** Toluene

**Synonyms:** Methacide; Methylbenzene; Methylbenzol; Phenylmethane; Toluol **Company Identification:**

VEE GEE Scientific, Inc. 13600 NE 126th Pl Ste A Kirkland, WA 98034

**For information in North America, call:** 425-823-4518

## Section 2 - Composition, Information on Ingredients

| CAS# | Chemical Name | Percent | EINECS/ELINCS |
|---|---|---|---|
| 108-88-3 | Toluene | >99 | 203-625-9 |

**Hazard Symbols:** XN F
**Risk Phrases:** 11 20

## Section 3 - Hazards Identification

### Emergency Overview

**Appearance:** Colorless. Flash Point: 40°F. **Warning!** Flammable liquid and vapor. May cause central nervous system depression. May cause liver and kidney damage. This substance has caused adverse reproductive and fetal effects in animals. Causes digestive and respiratory tract irritation. May cause skin irritation. Aspiration hazard if swallowed. Can enter lungs and cause damage. **Danger!** Harmful or fatal if swallowed. Causes eye irritation and possible transient injury. **Poison!** May be absorbed through intact skin. Vapor harmful. Call physician immmediately.
**Target Organs:** Kidneys, central nervous system, liver.
**Potential Health Effects**
**Eye Contact:** Causes eye irritation. May result in corneal injury. Vapors may cause eye irritation.
**Skin Contact:** Causes moderate skin irritation. May cause cyanosis of the extremities.
**Ingestion:** Aspiration hazard. May cause irritation of the digestive tract. May cause effects similar to those for inhalation exposure. Aspiration of material into the lungs may cause chemical pneumonitis, which may be fatal.
**Inhalation:** Inhalation of high concentrations may cause central nervous system effects characterized by nausea, headache, dizziness, unconsciousness and coma. Inhalation of vapor may cause respiratory tract irritation. May cause liver and kidney damage. Vapors may cause dizziness or suffocation. Overexposure may cause dizziness, tremors, restlessness, rapid heart beat, increased blood pressure, hallucinations, acidosis, kidney failure.
**Chronic Exposure:** Prolonged or repeated skin contact may cause dermatitis. May cause cardiac sensitization and severe heart abnormalities. May cause liver and kidney damage.

## Section 4 - First Aid Measures

**Eye Contact:** Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.
**Skin Contact:** Flush skin with plenty of soap and water for at least 15 minutes while removing contaminated clothing and shoes. Get medical aid if irritation develops or persists.
**Ingestion:** Do NOT induce vomiting. If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Possible aspiration hazard. Get medical aid immediately.
**Inhalation:** Get medical aid immediately. Remove from exposure to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.
**Notes to Physician:** Causes cardiac sensitization to endogenous catelcholamines which may lead to cardiac arrhythmias. Do NOT use adrenergic agents such as epinephrine or pseudoepinephrine.

## Section 5 - Fire Fighting Measures

**General Information:** Containers can build up pressure if exposed to heat and/or fire. As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Water runoff can cause environmental damage. Dike and collect water used to fight fire. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. Flammable Liquid. Can release vapors that form explosive mixtures at temperatures above the flashpoint. Use water spray to keep fire-exposed containers cool. Water may be ineffective. Material is lighter than water and a fire may be spread by the use of water. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas. Containers may explode when heated.
**Fire Extinguishing Media:** Use water spray to cool fire-exposed containers. Water may be ineffective. Do NOT use straight streams of water. For small fires, use dry chemical, carbon dioxide, water spray or regular foam. Cool containers with flooding quantities of water until well after fire is out. For large fires, use water spray, fog or regular foam.

## Section 5 - Fire Fighting Measures

**Autoignition Temperature:** 422°C (792°F)
**Flash Point:** 7°C (45°F)
**Explosion Limits, lower:** 1.2 vol%.
**Explosion Limits, upper:** 7.1 vol%
**NFPA Rating:** (estimated) Health: 2; Flammability: 3; Instability: 0

## Section 6 - Accidental Release Measures

**General Information:** Use proper personal protective equipment as indicated in Section 8.

**Spills/Leaks:** Avoid runoff into storm sewers and ditches which lead to waterways. Remove all sources of ignition. Absorb spill using an absorbent, non-combustible material such as earth, sand, or vermiculite. Do not use combustible materials such as saw dust. A vapor suppressing foam may be used to reduce vapors. Water spray may reduce vapor but may not prevent ignition in closed spaces.

## Section 7 - Handling and Storage

**Handling:** Wash thoroughly after handling. Use with adequate ventilation. Ground and bond containers when transferring material. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Avoid contact with heat, sparks and flame. Avoid ingestion and inhalation. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames.
**Storage:** Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

## Section 8 - Exposure Controls, Personal Protection

| Chemical Name | ACGIH | NIOSH | OSHA - Final PELs | OSHA - Vacated Pels |
|---|---|---|---|---|
| Toluene | 50 ppm TWA | 100 ppm TWA<br>375 mg/m3 TWA<br>500 ppm IDLH | 200 ppm TWA<br>C 300 ppm | 100 ppm TWA<br>375 mg/m3 TWA<br>150 ppm STEL<br>560 mg/m3 STEL |

**Engineering Controls:** Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.
**Personal Protective Equipment**

**Eyes:** Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
**Skin:** Wear appropriate protective gloves to prevent skin exposure.
**Clothing:** Wear appropriate protective clothing to prevent skin exposure.
**Respirators:** Follow the OSHA respirator regulations found in 29CFR 1910.134 or European Standard EN 149. Always use a NIOSH or European Standard EN 149 approved respirator when necessary.

## Section 9 - Physical and Chemical Properties

**Physical State:** Clear liquid
**Appearance:** Colorless
**Odor:** Sweet, pleasant
**pH:** Not available

**Vapor Pressure:** 36.7 mm Hg @ 30° C
**Vapor Density:** 3.1
**Evaporation Rate:** 2.4
**Viscosity:** 0.59 cP @ 20° C

**Boiling Point:** 232° F
**Freezing/Melting Point:** -139° F
**Decomposition Temperature:** Not available
**Solubility:** Insoluble
**Specific Gravity/Density:** 0.9
**Molecular Formula:** C6H5CH3
**Molecular Weight:** 92.056

## Section 10 - Stability and Reactivity

**Chemical Stability:** Stable under normal temperatures and pressures.
**Conditions to Avoid:** Incompatible materials, ignition sources, excess heat.
**Incompatibilities with Other Materials:** Ntrogen tetroxide, nitric acid plus sulfuric acid, silver perchlorate, strong oxidizers, sodium difluoride.
**Hazardous Decomposition Products:** Carbon monoxide, carbon dioxide.
**Hazardous Polymerization:** Has not been reported.

## Section 11 - Toxilogical Information

**Carcinogenicity:**
**CAS# 108-88-3:**
**ACGIH:** A4 - Not Classifiable as a Human Carcinogen

## Section 11 - Toxilogical Information (continued)

**Epidemiology:** No information available.

**Teratogenicity:** Specific developmental abnormalities included craniofacial effects involving the nose and tongue, musculoskeletal effects, urogenital and metabolic effects in studies on mice and rats by the inhalation and oral routes of exposure. Some evidence of fetotoxicity with reduced fetal weight and retarded skeletal development has been reported in mice and rats.
**Reproductive Effects:** Effects on fertility such as abortion were reported in rabbits by inhalation. Paternal effects were noted in rats by inhalation. These effects involved the testes, sperm duct and epididymis.
**Neurotoxicity:** No information available.
**Mutagenicity:** No information available.

## Section 12 - Ecological Information

**Ecotoxicity:** No data available. Bluegill LC50=17 mg/L/24H Shrimp LC50=4.3 ppm/96H Fathead minnow LC50=36.2 mg/L/96HSunfish (fresh water) TLm=1180 mg/L/96H
**Environmental:** From soil, substance evaporates and is microbially biodegraded. In water, substance volatilizes and biodegrades.
**Physical:** Photochemically produced hydroxyl radicals degrade substance.
**Other:** None.

## Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
**RCRA P-Series:** None listed.

**RCRA U-Series:** CAS# 108-88-3: waste number U220.

## Section 14 - Transport Information

| | US DOT | Canada TDG |
|---|---|---|
| **Shipping Name** | Toluene | Toluene |
| **Hazard Class** | 3 | 3 (9.2) |
| **UN Number** | UN1294 | UN1294 |
| **Packing Group** | II | II |
| **Other** | | FP 4C |

## Section 15 - Regulatory Information

### US Federal

**TSCA:** CAS# 108-88-3 is listed on the TSCA inventory.

**Health & Safety Reporting List:** None of the chemicals are on the Health & Safety Reporting List.
CAS# 108-88-3: Effective Date: October 4, 1982; Sunset Date: October 4 , 1992
**Chemical Test Rules:** None of the chemicals in this product are under a Chemical Test Rule.
**Section 12b:** None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule: None of the chemicals in this material have a SNUR under TSCA.
**SARA:**
**Section 302 (RQ):** CAS# 108-88-3: final RQ = 1000 pounds (454 kg)
**Section 302 (TPQ):** None of the chemicals in this product have a TPQ.
**SARA Codes:** CAS # 108-88-3: acute, flammable.
**Section 313:** This material contains Toluene (CAS# 108-88-3, 99%),which is subject to the reporting requirements of Section 313 of SARA Title III and 40 CFR Part 373.
**Clean Air Act:** CAS# 108-88-3 is listed as a hazardous air pollutant (HAP). This material does not contain any Class 1 Ozone depletors. This material does not contain any Class 2 Ozone depletors.
**Clean Water Act:** CAS# 108-88-3 is listed as a Hazardous Substance under the CWA. CAS# 108-88-3 is listed as a Priority Pollutant under the Clean Water Act. CAS# 108-88-3 is listed as a Toxic Pollutant under the Clean Water Act.
**OSHA:** None of the chemicals in this product are considered highly hazardous by OSHA.

**STATE:** CAS# 108-88-3 can be found on the following state right to know lists: California, New Jersey, Florida, Pennsylvania, Minnesota, Massachusetts.
WARNING: This product contains Toluene, a chemical known to the state of California to cause birth defects or other reproductive harm. California No

Significant Risk Level: CAS# 108-88-3: NOEL = 7000 ug/day

### European/International Regulations

**European Labeling in Accordance with EC Directives**
**Hazard Symbols:** XN F
**Risk Phrases:**

R 11 Highly flammable.

R 20 Harmful by inhalation



## Section 15 - Regulatory Information (continued)

**Safety Phrases:**

S 16 Keep away from sources of ignition - No smoking. S 25 Avoid contact with eyes.
S 29 Do not empty into drains.

S 33 Take precautionary measures against static discharges.

**WGK (Water Danger/Protection):** CAS# 108-88-3: 2

**Canada - DSL/NDSL:** CAS# 108-88-3 is listed on Canada's DSL List.
**Canada - WHMIS:** This product has a WHMIS classification of B2, D2B.
**Canadian Ingredient Disclosure List:** CAS# 108-88-3 is listed on Canada's Ingredient Disclosure List.

**Exposure Limits:** CAS# 108-88-3: OEL-AUSTRALIA:TWA 100 ppm (375 mg/m3);STEL 150 ppm (560 mg/m3) OEL-BELGIUM:TWA 100 ppm (377 g/m3);STEL 150 ppm (565 mg/m3) OEL-CZECHOSLOVAKIA:TWA 200 mg/m3;STEL 1000 mg/m3 OEL-DENMARK:TWA 50 ppm (190 mg/m3);Skin OEL-FINLAND:TWA 100 ppm (375 mg/m3);STEL 150 ppm;Skin OEL-FRANCE:TWA 100 ppm (375 mg/m3);STEL 150 ppm (560 mg/m3) OEL-GERMANY:TWA 100 ppm (380 mg/m3) OEL-HUNGARY:TWA 100 mg/m3;STEL 300 mg/m3;Skin OEL-JAPAN:TWA 100 ppm (380 mg/m3) OEL-THE NETHERLANDS:TWA 100 ppm (375 mg/m3);Skin OEL-THE PHILIPPINES:TWA 100 ppm (375 mg/m3) OEL-POLAND:TWA 100 mg/m3 OEL-USSIA:TWA 100 ppm;STEL 50 mg/m3 OEL-SWEDEN:TWA 50 ppm (200 mg/m3);STEL 100 ppm (400 mg/m3);Skin OEL-SWITZERLAND:TWA 100 ppm (380 mg/m3);STEL 500 ppm OEL-THAILAND:TWA 200 ppm;STEL 300 ppm OEL-TURKEY:TWA 200 ppm (750 mg/m3) OEL-UNITED KINGDOM :TWA 100 ppm (375 mg/m3);STEL 150 ppm;Skin OEL IN BULGARIA, COLOMBIA,JORDAN, KOREA check ACGIH TLV OEL IN NEW ZEALAND, SINGAPORE, VIETNAM check ACGI TLV

## Section 16 - Additional Information

**MSDS Creation Date:** 09/07/2004

aT0470

TCI AMERICA

# Material Safety Data Sheet

| HAZARD WARNINGS | RISK PHRASES | PROTECTIVE CLOTHING |
|---|---|---|
| | Combustible material; avoid heat and sources of ignition.<br>Harmful compound, minimize exposure.<br>Irritating to skin, eyes, and the respiratory system.<br>Dangerous for the environment | |

## Section I. Chemical Product and Company Identification

| | |
|---|---|
| Chemical Name | 1,3,5-Trimethylbenzene |
| Catalog Number | T0470 |
| Synonym | Mesitylene |
| Chemical Formula | $(CH_3)_3C_6H_3$ |
| CAS Number | 108-67-8 |

Supplier: TCI America, 9211 N. Harborgate St., Portland OR, 1-800-423-8616

In case of Emergency Call: Chemtrec®, (800) 424-9300 (U.S.), (703) 527-3887 (International)

## Section II. Composition and Information on Ingredients

| Chemical Name | CAS Number | Percent (%) | TLV/PEL | Toxicology Data |
|---|---|---|---|---|
| 1,3,5-Trimethylbenzene | 108-67-8 | Min. 97.0 (GC) | Not available. | Rat $LC_{50}$ (inhalation) 24gm/$m^3$/4H |

## Section III. Hazards Identification

**Acute Health Effects**

Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.
Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

**Chronic Health Effects**

CARCINOGENIC EFFECTS : Not available.
MUTAGENIC EFFECTS : Not available.
TERATOGENIC EFFECTS : Not available.
DEVELOPMENTAL TOXICITYNot available.
Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

## Section IV. 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. Get medical attention.

**Skin Contact**

In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

**Inhalation**

If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.

**Ingestion**

INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. SEEK IMMEDIATE MEDICAL ATTENTION in case of ingestion of a radioactive material.

## Section V. Fire and Explosion Data

| | | | |
|---|---|---|---|
| Flammability | Combustible. | Auto-Ignition | Not available. |
| | | | LOWER: 0.88% |

| | | | |
|---|---|---|---|
| Flash Points | 44.44°C (112°F). | Flammable Limits | |
| Combustion Products | These products are toxic carbon oxides (CO, $CO_2$). | | |
| Fire Hazards | Risks of explosion of the product in presence of mechanical impact: Not available.<br>Risks of explosion of the product in presence of static discharge: Not available. | | |
| Explosion Hazards | Combustible liquid.<br>SMALL FIRE: Use DRY chemical powder. | | |
| Fire Fighting Media | 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. Consult with local fire authorities before attempting large scale fire fighting operations. | | |

3/11/2005.

| | |
|---|---|
| Acute Toxic Effects | Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. |





## Section XII. Ecological Information

| | |
|---|---|
| Ecotoxicity | Toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment. |
| Environmental Fate | Mesitylene's production and use as a dyestuff intermediate, solvent, paint thinner, and as a UV oxidation stabilizer for plastics may result in its release to the environment through various waste streams. Mesitylene is released directly to the environment as a component of gasoline and as an emission from gasoline-powered vehicles, municipal waste-treatment plants, and coal-fired power stations. If released to the atmosphere, mesitylene will exist solely in the vapor phase in the ambient atmosphere, based on a measured vapor pressure of 2.48 mm Hg at 25 deg C. Vapor-phase mesitylene is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and nitrate radicals with half-lives of about 7 hours and 10-67 days, respectively. A measured Koc value of 660 suggests that mesitylene will have low mobility in soil. Volatilization from moist and dry soil surfaces should occur based on a measured Henry's Law constant of 8.77X10-3 atm-cu m/mole and the vapor pressure of this compound, respectively. Mesitylene should aerobically biodegrade in both soil and water. Mesitylene was not degraded in methanogenic aquifer microcosms. In water, mesitylene may adsorb to sediment or particulate matter based on its Koc value. This compound should volatilize from water surfaces given its Henry's Law constant. Estimated half-lives for a model river and model lake are 3 hours and 4 days, respectively. Bioconcentration in aquatic organisms may occur based on BCF values of 23-342, measured in carp. The general population will be exposed to mesitylene via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with vapors, food and other products containing mesitylene. Occupational exposure may occur through inhalation and dermal contact with this compound at workplaces where it is produced or used. |

## Section XIII. Disposal Considerations

| | |
|---|---|
| Waste Disposal | Recycle to process, if possible. Consult your local regional authorities. You may be able to dissove or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and locl regulations when disposing of the substance. |

## Section XIV. sport Information

| | |
|---|---|
| DOT Classification | CLASS 3: Flammable liquid. |
| PIN Number | UN2325 |
| Proper Shipping Name | 1,3,5-Trimethylbenzene |
| Packing Group (PG) | III |
| DOT Pictograms |  |

## Section XV. Other Regulatory Information and Pictograms

| | |
|---|---|
| TSCA Chemical Inventory (EPA) | This compound is ON the EPA Toxic Substances Control Act (TSCA) inventory list. |
| WHMIS Classification (Canada) | CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F). This product is subject to SARA section 313 reporting requirements (8a PAIR). |
| EINECS Number (EEC) | 203-604-4 |
| EEC Risk Statements | R20/21/22- Harmful by inhalation, in contact with skin and if swallowed. R36/37/38- Irritating to eyes, respiratory system and skin. R51- Toxic to aquatic organisms. R53- May cause long-term adverse effects in the aquatic environment. |
| Japanese Regulatory Data | Not available. |

## Section XVI. Other Information

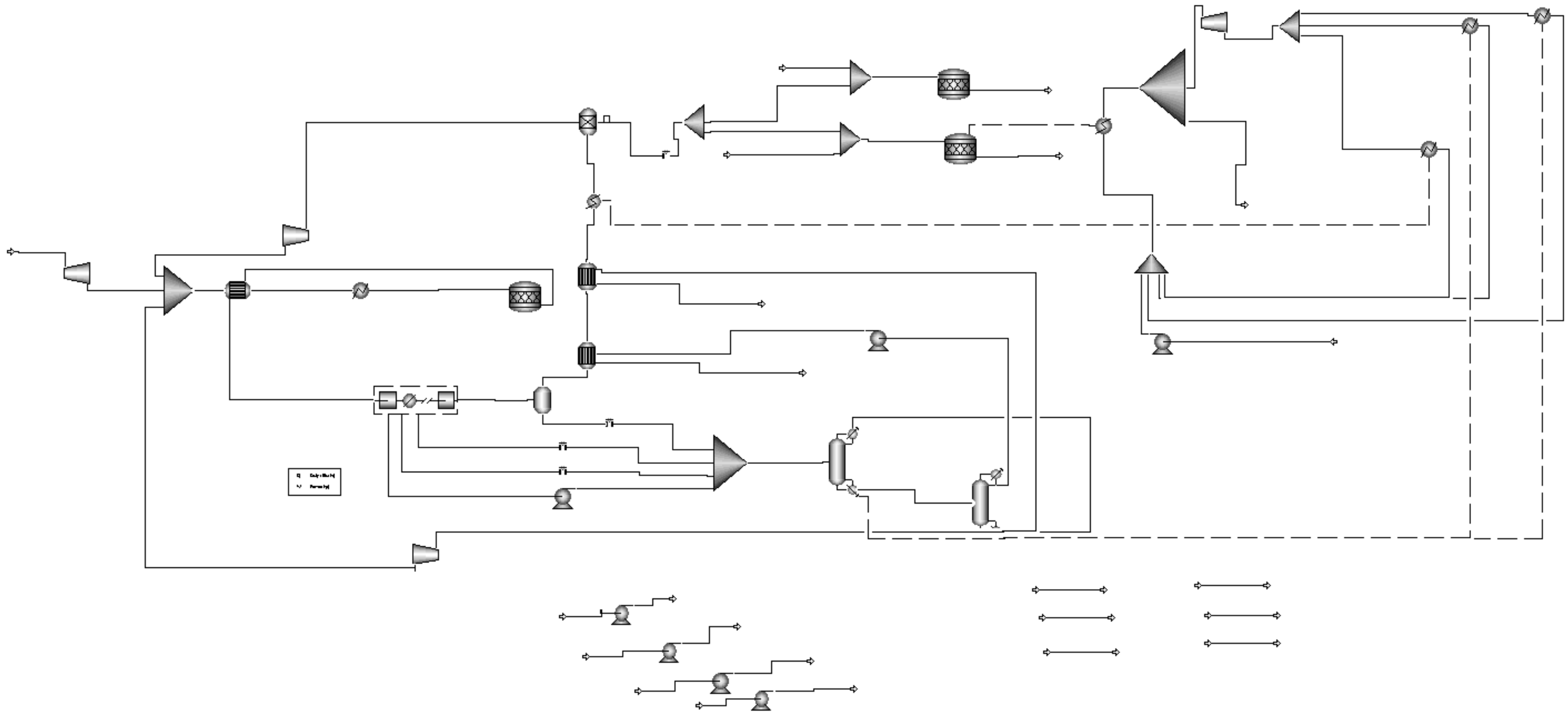
Version 1.0

Validated on 6/7/2002.
Printed 3/11/2005.

Notice to Reader

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. 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 chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local

# A-5. ASPEN Data



## *A-5.1. Input File*

```
;
;Input Summary created by Aspen Plus Rel. 32.0 at 17:36:27 Sat Apr 11, 2015
;Directory  S:\Documents\CBE  459\New  Catalyst  L  ver2-6-1_1    Filename
C:\Users\jlym\AppData\Local\Temp\~ap972.txt
;


DYNAMICS
    DYNAMICS RESULTS=ON

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

MODEL-OPTION

DATABANKS 'APV86 PURE32' / 'APV86 AQUEOUS' / 'APV86 SOLIDS' /  &
        'APV86 INORGANIC' / NOASPENPCD

PROP-SOURCES 'APV86 PURE32' / 'APV86 AQUEOUS' / 'APV86 SOLIDS' &
         / 'APV86 INORGANIC'

COMPONENTS
    HYDROGEN H2 /
    METHANE CH4 /
    ETHANE C2H6 /
    ETHENE C2H4 /
    PROPANE C3H8 /
    PROPENE C3H6-2 /
    BENZENE C6H6 /
    TOLUENE C7H8 /
    P-XYL-01 C8H10-3 /
    1:3:5-01 C9H12-8 /
    WATER H2O /
    OXYGEN O2 /
    NITROGEN N2 /
    CARBO-01 CO2

SOLVE
    RUN-MODE MODE=SIM

FLOWSHEET
    BLOCK R-101 IN=S-106, OUT=S-107
    BLOCK F-101, IN=S-106 OUT=S-106,
    BLOCK F-101 IN=S-220, OUT=S-110
    BLOCK V-103 IN=S-109 S-220 OUT=S-220,
    BLOCK V-203-5 IN=S-209 S-208 S-207 S-206 OUT=S-210
    BLOCK P-201 IN=S-204 OUT=S-209
    BLOCK PR-201 IN=S-214 OUT=S-219, S-218
    BLOCK V-101-2 IN=S-102 S-104 S-103 OUT=S-105
    BLOCK V-206 IN=S-219 OUT=S-221 S-220
    BLOCK T-105 IN=S-305 OUT=S-104
    BLOCK T-104 IN=S-101 OUT=S-102
    BLOCK COL-301 IN=S-210 OUT=S-305 S-310 HEAT3
```

```
    BLOCK F-401-2 IN=S-221, OUT=S-411 HEAT1
    BLOCK V-404 IN=S-221 S-410 OUT=S-221,
    BLOCK H-101 IN=S-107 S-105 OUT=S-108 S-106
    BLOCK COL-302 IN=S-310 OUT=S-315 S-320 HEAT4
    BLOCK V-201 IN=S-205 OUT=S-206
    BLOCK V-203 IN=S-203 OUT=S-208
    BLOCK V-202 IN=S-202 OUT=S-207
    BLOCK C-201-3 IN=S-108 OUT=S-201 S-204 S-203 S-202
    BLOCK F-401-2, IN=S-403 HEAT1 OUT=S-404
    BLOCK V-405 IN=S-404 OUT=S-405 S-406
    BLOCK RB-301 IN=S-408 HEAT3 OUT=S-308
    BLOCK RB-302 IN=S-409 HEAT4 OUT=S-319
    BLOCK H-201 IN=S-222 S-211 OUT=S-215 S-212
    BLOCK H-203 IN=S-213 OUT=S-214 HEAT2
    BLOCK H-202 IN=S-320 S-212 OUT=S-216 S-213
    BLOCK T-101-3 IN=S-218 OUT=S-103
    BLOCK COL-201 IN=S-201 OUT=S-211 S-205
    BLOCK H-203, IN=S-407 HEAT2 OUT=S-217
    BLOCK PR-201, IN=S-219, OUT=S-219
    BLOCK V-401-3 IN=S-402 S-319 S-217 S-308 OUT=S-403
    BLOCK P-401 IN=S-401 OUT=S-402
    BLOCK T-401 IN=S-406 OUT=S-406,
    BLOCK V-406-7 IN=S-406, OUT=S-408 S-409 S-407
    BLOCK P-301 IN=S-303 OUT=S-304
    BLOCK P-302 IN=S-306 OUT=S-307
    BLOCK P-303 IN=S-313 OUT=S-314
    BLOCK P-304 IN=S-316 OUT=S-317
    BLOCK P-202 IN=S-315 OUT=S-222

PROPERTIES NRTL-RK

PROP-DATA NRTL-1
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar'
    PROP-LIST NRTL
    BPVAL PROPENE BENZENE 0.0 178.8998000 .3000000000 0.0 0.0  &
        0.0 25.00000000 25.00000000
    BPVAL BENZENE PROPENE 0.0 46.73830000 .3000000000 0.0 0.0  &
        0.0 25.00000000 25.00000000
    BPVAL BENZENE TOLUENE -2.719200000 1083.397500 .3000000000  &
        0.0 0.0 0.0 40.00000000 110.7500000
    BPVAL TOLUENE BENZENE 2.067100000 -831.3335000 .3000000000  &
        0.0 0.0 0.0 40.00000000 110.7500000
    BPVAL BENZENE P-XYL-01 0.0 222.4249000 .3000000000 0.0 0.0  &
        0.0 83.60000000 129.0000000
    BPVAL P-XYL-01 BENZENE 0.0 -197.7876000 .3000000000 0.0  &
        0.0 0.0 83.60000000 129.0000000
    BPVAL TOLUENE P-XYL-01 0.0 -114.6844000 .3000000000 0.0  &
        0.0 0.0 111.2300000 137.1000000
    BPVAL P-XYL-01 TOLUENE 0.0 107.5213000 .3000000000 0.0 0.0  &
        0.0 111.2300000 137.1000000
    BPVAL BENZENE WATER 45.19050000 591.3676000 .2000000000 0.0  &
        -7.562900000 0.0 .8000000000 77.00000000
    BPVAL WATER BENZENE 140.0874000 -5954.307100 .2000000000  &
        0.0 -20.02540000 0.0 .8000000000 77.00000000
    BPVAL TOLUENE WATER -247.8792000 14759.75980 .2000000000  &
        0.0 35.58200000 0.0 -9.000000000 93.00000000
```

```
    BPVAL WATER TOLUENE 627.0528000 -27269.35550 .2000000000  &
        0.0 -92.71820000 0.0 -9.000000000 93.00000000
    BPVAL P-XYL-01 WATER 2.773400000 296.6645000 .2000000000  &
        0.0 .1174000000 0.0 0.0 294.9000000
    BPVAL WATER P-XYL-01 162.4774000 -6045.999500 .2000000000  &
        0.0 -23.46720000 0.0 0.0 294.9000000
    BPVAL 1:3:5-01 WATER -3.726400000 2542.779300 .2000000000  &
        0.0 0.0 0.0 20.00000000 40.00000000
    BPVAL WATER 1:3:5-01 10.25210000 -66.03660000 .2000000000  &
        0.0 0.0 0.0 20.00000000 40.00000000
    BPVAL WATER CARBO-01 10.06400000 -3268.135000 .2000000000  &
        0.0 0.0 0.0 0.0 200.0000000
    BPVAL CARBO-01 WATER 10.06400000 -3268.135000 .2000000000  &
        0.0 0.0 0.0 0.0 200.0000000

STREAM S-101
    SUBSTREAM MIXED TEMP=80.00000000 PRES=264.6959487  &
        MASS-FLOW=5707.767968
    MOLE-FRAC METHANE 0.01 / ETHANE 0.97 / PROPANE 0.02

STREAM S-109
    SUBSTREAM MIXED TEMP=77.00000000 PRES=14.50377377  &
        MOLE-FLOW=22046.22622
    MOLE-FRAC OXYGEN 0.21 / NITROGEN 0.79

STREAM S-301
    SUBSTREAM MIXED TEMP=209.392 PRES=93. MASS-FLOW=22552.844  &
        FREE-WATER=NO NPHASE=1 PHASE=V
    MASS-FRAC HYDROGEN 4.57E-009 / METHANE 0.120733261 /  &
        ETHANE 0.31430703 / ETHENE 0.027124142 / PROPANE  &
        0.031919275 / PROPENE 0.006390641 / BENZENE  &
        0.445045079 / TOLUENE 0.052578284 / P-XYL-01  &
        0.001899723 / 1:3:5-01 2.56E-006 / WATER 0. / OXYGEN  &
        0. / NITROGEN 0. / CARBO-01 0.

STREAM S-302
    SUBSTREAM MIXED TEMP=186.1 VFRAC=0.897120543  &
        MASS-FLOW=22552.844
    MASS-FRAC HYDROGEN 4.57E-009 / METHANE 0.120733261 /  &
        ETHANE 0.31430703 / ETHENE 0.027124142 / PROPANE  &
        0.031919275 / PROPENE 0.006390641 / BENZENE  &
        0.445045079 / TOLUENE 0.052578284 / P-XYL-01  &
        0.001899723 / 1:3:5-01 2.56E-006

STREAM S-303
    SUBSTREAM MIXED TEMP=186.1 PRES=83. MASS-FLOW=2103.78883  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC HYDROGEN 2.21E-016 / METHANE 0.002560832 /  &
        ETHANE 0.024119202 / ETHENE 0.001717492 / PROPANE  &
        0.004315422 / PROPENE 0.000507373 / BENZENE  &
        0.790953211 / TOLUENE 0.166730683 / P-XYL-01  &
        0.009080698 / 1:3:5-01 1.51E-005

STREAM S-306
    SUBSTREAM MIXED TEMP=339.938 PRES=102.3 MASS-FLOW=264044.408  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC HYDROGEN 2.33E-274 / METHANE 3.23E-067 / ETHANE  &
```

```
        2.39E-024 / ETHENE 9.62E-028 / PROPANE 2.2E-017 /  &
        PROPENE 3.29E-026 / BENZENE 0.660110215 / TOLUENE  &
        0.233327963 / P-XYL-01 0.050159506 / 1:3:5-01  &
        0.056402315

STREAM S-309
    SUBSTREAM MIXED TEMP=348.53 PRES=102.45 MASS-FLOW=138213.865  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC HYDROGEN 4.45E-274 / METHANE 6.1E-067 / ETHANE  &
        4.14E-024 / ETHENE 1.68E-027 / PROPANE 3.63E-017 /  &
        PROPENE 5.67E-026 / BENZENE 0.752673327 / TOLUENE  &
        0.194888485 / P-XYL-01 0.029617377 / 1:3:5-01  &
        0.022820812

STREAM S-311
    SUBSTREAM MIXED TEMP=241.229 PRES=26. MASS-FLOW=187342.041  &
        FREE-WATER=NO NPHASE=1 PHASE=V
    MASS-FRAC BENZENE 0.615754339 / TOLUENE 0.303831852 /  &
        P-XYL-01 0.080058695 / 1:3:5-01 0.000355114

STREAM S-312
    SUBSTREAM MIXED TEMP=196.384 PRES=16. MASS-FLOW=187342.041  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC BENZENE 0.615754339 / TOLUENE 0.303831852 /  &
        P-XYL-01 0.080058695 / 1:3:5-01 0.000355114

STREAM S-313
    SUBSTREAM MIXED TEMP=196.384 PRES=16. MASS-FLOW=114117.806  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC BENZENE 0.615754339 / TOLUENE 0.303831852 /  &
        P-XYL-01 0.080058695 / 1:3:5-01 0.000355114

STREAM S-316
    SUBSTREAM MIXED TEMP=386.837 PRES=31.85 MASS-FLOW=194453.214  &
        FREE-WATER=NO NPHASE=1 PHASE=L
    MASS-FRAC BENZENE 8.08E-011 / TOLUENE 9.14E-007 /  &
        P-XYL-01 0.002075488 / 1:3:5-01 0.997923598

STREAM S-318
    SUBSTREAM MIXED TEMP=387.281 PRES=32. MASS-FLOW=182740.516  &
        FREE-WATER=NO NPHASE=1 PHASE=V
    MASS-FRAC HYDROGEN 0. / METHANE 0. / ETHANE 0. /  &
        ETHENE 0. / PROPANE 0. / PROPENE 0. / BENZENE  &
        8.49E-011 / TOLUENE 9.52E-007 / P-XYL-01 0.002128228 /  &
        1:3:5-01 0.99787082 / WATER 0. / OXYGEN 0. /  &
        NITROGEN 0. / CARBO-01 0.

STREAM S-401
    SUBSTREAM MIXED TEMP=77.00000000 PRES=14.50377377  &
        MASS-FLOW=1.03970664E+6
    MASS-FRAC WATER 1.

STREAM S-410
    SUBSTREAM MIXED TEMP=77.00000000 PRES=14.50377377  &
        MOLE-FLOW=2.20462262E+5
    MOLE-FRAC OXYGEN 0.21 / NITROGEN 0.79
```

```
DEF-STREAMS HEAT HEAT1

DEF-STREAMS HEAT HEAT2

DEF-STREAMS HEAT HEAT3

DEF-STREAMS HEAT HEAT4

BLOCK V-101-2 MIXER
    PARAM

BLOCK V-103 MIXER
    PARAM

BLOCK V-203-5 MIXER
    PARAM

BLOCK V-401-3 MIXER
    PARAM

BLOCK V-404 MIXER
    PARAM

BLOCK V-206 FSPLIT
    FRAC S-221 0.

;0.014605878
; 0.016515892

BLOCK V-405 FSPLIT
    FRAC S-406 0.071210559

BLOCK V-406-7 FSPLIT
    FRAC S-408 0.329935017 / S-409 0.431538716

BLOCK PR-201 SEP
    PARAM PRES=-10.00000000
    FRAC STREAM=S-219, SUBSTREAM=MIXED COMPS=HYDROGEN METHANE  &
        ETHANE ETHENE PROPANE PROPENE BENZENE TOLUENE P-XYL-01  &
        1:3:5-01 WATER OXYGEN NITROGEN CARBO-01 FRACS=0.85  &
        0.28 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.

BLOCK F-101, HEATER
    PARAM TEMP=1166.000000 PRES=0.0

BLOCK F-401-2, HEATER
    PARAM PRES=450. <psig> NPHASE=2 TOL=0.0001 T-EST=384.2600000
    BLOCK-OPTION FREE-WATER=NO

BLOCK H-203 HEATER
    PARAM TEMP=181.4000000 PRES=-10.00000000

BLOCK H-203, HEATER
    PARAM PRES=-10.00000000

BLOCK RB-301 HEATER
    PARAM PRES=-10.00000000 NPHASE=2
```

```
    BLOCK-OPTION FREE-WATER=NO

BLOCK RB-302 HEATER
    PARAM PRES=-10.00000000 NPHASE=2
    BLOCK-OPTION FREE-WATER=NO

BLOCK COL-201 FLASH2
    PARAM TEMP=104.0000000 PRES=0.0 TOL=0.0001

BLOCK H-101 HEATX
    PARAM DELT-COLD=18. CALC-TYPE=DESIGN PRES-HOT=-10.00000000  &
        PRES-COLD=-10.00000000 MIN-TAPP=18.00000000 U-OPTION=PHASE  &
        F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=S-107 COLD=S-105
    OUTLETS-HOT S-108
    OUTLETS-COLD S-106
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT
    TQ-PARAM CURVE=YES

BLOCK H-201 HEATX
    PARAM DELT-HOT=18. <C> CALC-TYPE=DESIGN  &
        PRES-HOT=-10.00000000 PRES-COLD=-10.00000000  &
        MIN-TAPP=18.00000000 U-OPTION=PHASE F-OPTION=CONSTANT  &
        CALC-METHOD=SHORTCUT
    FEEDS HOT=S-222 COLD=S-211
    OUTLETS-HOT S-215
    OUTLETS-COLD S-212
    HOT-SIDE DP-OPTION=CONSTANT
    COLD-SIDE DP-OPTION=CONSTANT
    TQ-PARAM CURVE=YES

BLOCK H-202 HEATX
    PARAM DELT-HOT=10. <C> CALC-TYPE=DESIGN  &
        PRES-HOT=-10.00000000 PRES-COLD=-10.00000000  &
        U-OPTION=PHASE F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=S-320 COLD=S-212
    OUTLETS-HOT S-216
    OUTLETS-COLD S-213
    HOT-SIDE DP-OPTION=CONSTANT
    COLD-SIDE DP-OPTION=CONSTANT
    TQ-PARAM CURVE=YES

BLOCK COL-301 RADFRAC
    PARAM NSTAGE=65 ALGORITHM=STANDARD EFF=MURPHREE MAXOL=25  &
        DAMPING=NONE
    COL-CONFIG CONDENSER=PARTIAL-V
    RATESEP-ENAB CALC-MODE=EQUILIBRIUM
    FEEDS S-210 22
    PRODUCTS S-305 1 V / S-310 65 L
    PRODUCTS HEAT3 65
    P-SPEC 1 83.
    COL-SPECS MASS-D:F=0.089716729 DP-STAGE=0.15  &
        MASS-RR=0.10287944 DP-COND=10.
    STEFF-SEC SECNO=1 1 65 0.65

BLOCK COL-302 RADFRAC
```

```
    PARAM NSTAGE=42 ALGORITHM=STANDARD EFF=MURPHREE MAXOL=25  &
        DAMPING=NONE
    COL-CONFIG CONDENSER=TOTAL
    FEEDS S-310 23
    PRODUCTS S-315 1 L / S-320 42 L
    PRODUCTS HEAT4 42
    P-SPEC 1 16.
    COL-SPECS MASS-D:F=0.906916873 DP-STAGE=0.15  &
        MASS-RR=0.641654779 DP-COND=10.
    STEFF-SEC SECNO=1 1 42 0.65

BLOCK F-101 RSTOIC
    PARAM TEMP=1346.000000 PRES=14.50377377 HEAT-OF-REAC=YES
    STOIC 1 MIXED METHANE -1. / OXYGEN -2. / CARBO-01 1. /  &
        WATER 2.
    STOIC 2 MIXED ETHANE -2. / OXYGEN -7. / CARBO-01 4. /  &
        WATER 6.
    STOIC 3 MIXED PROPANE -1. / OXYGEN -5. / CARBO-01 3. /  &
        WATER 4.
    STOIC 4 MIXED HYDROGEN -2. / OXYGEN -1. / WATER 2.
    CONV 1 MIXED METHANE 1.
    CONV 2 MIXED ETHANE 1.
    CONV 3 MIXED PROPANE 1.
    CONV 4 MIXED HYDROGEN 1.
    HEAT-RXN REACNO=1 CID=METHANE / REACNO=2 CID=ETHANE /  &
        REACNO=3 CID=PROPANE / REACNO=4 CID=HYDROGEN

BLOCK F-401-2 RSTOIC
    PARAM TEMP=572.0000000 PRES=14.50377377 HEAT-OF-REAC=YES
    STOIC 1 MIXED METHANE -1. / OXYGEN -2. / CARBO-01 1. /  &
        WATER 2.
    STOIC 2 MIXED HYDROGEN -2. / OXYGEN -1. / WATER 2.
    CONV 1 MIXED METHANE 1.
    CONV 2 MIXED HYDROGEN 1.
    HEAT-RXN REACNO=1 CID=METHANE / REACNO=2 CID=HYDROGEN

BLOCK R-101 RSTOIC
    PARAM TEMP=1166.000000 PRES=-7.251886887 SERIES=NO  &
        HEAT-OF-REAC=YES
    STOIC 1 MIXED ETHANE -1. / HYDROGEN -1. / METHANE 2.
    STOIC 2 MIXED ETHANE -1. / ETHENE 1. / HYDROGEN 1.
    STOIC 3 MIXED ETHANE -3. / PROPENE 2. / HYDROGEN 3.
    STOIC 4 MIXED ETHANE -3. / PROPANE 2. / HYDROGEN 1.
    STOIC 5 MIXED ETHANE -3. / BENZENE 1. / HYDROGEN 6.
    STOIC 6 MIXED ETHANE -4. / TOLUENE 1. / METHANE 1. /  &
        HYDROGEN 6.
    STOIC 7 MIXED ETHANE -4. / P-XYL-01 1. / HYDROGEN 7.
    STOIC 8 MIXED ETHANE -5. / 1:3:5-01 1. / METHANE 1. /  &
        HYDROGEN 7.
    STOIC 9 MIXED ETHENE -1. / HYDROGEN -2. / METHANE 2.
    STOIC 10 MIXED ETHENE -3. / PROPENE 2.
    STOIC 11 MIXED ETHENE -3. / HYDROGEN -2. / PROPANE 2.
    STOIC 12 MIXED ETHENE -3. / BENZENE 1. / HYDROGEN 3.
    STOIC 13 MIXED ETHENE -4. / TOLUENE 1. / HYDROGEN 2. /  &
        METHANE 1.
    STOIC 14 MIXED ETHENE -4. / P-XYL-01 1. / HYDROGEN 3.
    STOIC 15 MIXED ETHENE -5. / 1:3:5-01 1. / HYDROGEN 2. /  &
```

```
    METHANE 1.
STOIC 16 MIXED PROPANE -2. / BENZENE 1. / HYDROGEN 5.
STOIC 17 MIXED PROPANE -3. / TOLUENE 1. / ETHANE 1. /  &
    HYDROGEN 5.
STOIC 18 MIXED PROPANE -3. / P-XYL-01 1. / METHANE 1. /  &
    HYDROGEN 5.
STOIC 19 MIXED PROPENE -1. / HYDROGEN -1. / METHANE 1. / &
    ETHENE 1.
STOIC 20 MIXED PROPENE -2. / BENZENE 1. / HYDROGEN 3.
STOIC 21 MIXED PROPENE -3. / TOLUENE 1. / ETHANE 1. /  &
    HYDROGEN 2.
STOIC 22 MIXED PROPENE -3. / P-XYL-01 1. / METHANE 1. /  &
    HYDROGEN 2.
STOIC 23 MIXED PROPANE -3. / 1:3:5-01 1. / HYDROGEN 6.
STOIC 24 MIXED PROPENE -3. / 1:3:5-01 1. / HYDROGEN 3.
CONV 1 MIXED ETHANE 0.07582
CONV 2 MIXED ETHANE 0.05904
CONV 3 MIXED ETHANE 0.00718
CONV 4 MIXED ETHANE 0.00685
CONV 5 MIXED ETHANE 0.17372
CONV 6 MIXED ETHANE 0.0925
CONV 7 MIXED ETHANE 0.01934
CONV 8 MIXED ETHANE 0.02982
CONV 9 MIXED ETHENE 0.1871
CONV 10 MIXED ETHENE 0.0177
CONV 11 MIXED ETHENE 0.0169
CONV 12 MIXED ETHENE 0.4287
CONV 13 MIXED ETHENE 0.2283
CONV 14 MIXED ETHENE 0.0477
CONV 15 MIXED ETHENE 0.0736
CONV 16 MIXED PROPANE 0.18153
CONV 17 MIXED PROPANE 0.2333
CONV 18 MIXED PROPANE 0.1037
CONV 19 MIXED PROPENE 0.3487
CONV 20 MIXED PROPENE 0.228
CONV 21 MIXED PROPENE 0.2931
CONV 22 MIXED PROPENE 0.1303
CONV 23 MIXED PROPANE 0.064656
CONV 24 MIXED PROPENE 0.08119
HEAT-RXN REACNO=1 CID=ETHANE TEMP=1166.000000 / REACNO=2  &
    CID=ETHANE TEMP=1166.000000 / REACNO=3 CID=ETHANE  &
    TEMP=1166.000000 / REACNO=4 CID=ETHANE TEMP=1166.000000 /  &
    REACNO=5 CID=ETHANE TEMP=1166.000000 / REACNO=6  &
    CID=ETHANE TEMP=1166.000000 / REACNO=7 CID=ETHANE  &
    TEMP=1166.000000 / REACNO=8 CID=ETHANE TEMP=1166.000000 /  &
    REACNO=9 CID=ETHENE TEMP=1166.000000 / REACNO=10  &
    CID=ETHENE TEMP=1166.000000 / REACNO=11 CID=ETHENE  &
    TEMP=1166.000000 / REACNO=12 CID=ETHENE TEMP=1166.000000 / &
    REACNO=13 CID=ETHENE TEMP=1166.000000 / REACNO=14  &
    CID=ETHENE TEMP=1166.000000 / REACNO=15 CID=ETHENE  &
    TEMP=1166.000000 / REACNO=16 CID=PROPANE  &
    TEMP=1166.000000 / REACNO=17 CID=PROPANE  &
    TEMP=1166.000000 / REACNO=18 CID=PROPANE  &
    TEMP=1166.000000 / REACNO=19 CID=PROPENE  &
    TEMP=1166.000000 / REACNO=20 CID=PROPENE  &
    TEMP=1166.000000 / REACNO=21 CID=PROPENE  &
    TEMP=1166.000000 / REACNO=22 CID=PROPENE  &
```

```
        TEMP=1166.000000 / REACNO=23 CID=PROPANE  &
        TEMP=1166.000000 / REACNO=24 CID=PROPENE  &
        TEMP=1166.000000

BLOCK P-201 PUMP
    PARAM PRES=100. EFF=0.8

BLOCK P-202 PUMP
    PARAM DELP=10. EFF=0.8

BLOCK P-301 PUMP
    PARAM PRES=93. EFF=0.8

BLOCK P-302 PUMP
    PARAM PRES=109. EFF=0.8

BLOCK P-303 PUMP
    PARAM PRES=45. EFF=0.8

BLOCK P-304 PUMP
    PARAM DELP=10. EFF=0.8

BLOCK P-401 PUMP
    PARAM PRES=230. EFF=0.8

BLOCK T-101-3 COMPR
    PARAM TYPE=ISENTROPIC PRES=53.66396296 SEFF=0.8 NPHASE=2  &
        SB-MAXIT=30 SB-TOL=0.0001  MODEL-TYPE=TURBINE
    BLOCK-OPTION FREE-WATER=NO

BLOCK T-104 COMPR
    PARAM TYPE=ISENTROPIC PRES=53.66396296 SEFF=0.8 NPHASE=2  &
        SB-MAXIT=30 SB-TOL=0.0001  MODEL-TYPE=TURBINE
    BLOCK-OPTION FREE-WATER=NO

BLOCK T-105 COMPR
    PARAM TYPE=ISENTROPIC PRES=53.66396296 SEFF=0.8 NPHASE=2  &
        SB-MAXIT=30 SB-TOL=0.0001  MODEL-TYPE=TURBINE
    BLOCK-OPTION FREE-WATER=NO

BLOCK T-401 COMPR
    PARAM TYPE=ISENTROPIC PRES=240. SEFF=0.8 NPHASE=2  &
        SB-MAXIT=30 SB-TOL=0.0001  MODEL-TYPE=TURBINE
    BLOCK-OPTION FREE-WATER=NO

BLOCK C-201-3 MCOMPR
    PARAM NSTAGE=4 TYPE=ISENTROPIC SB-MAXIT=30 SB-TOL=0.0001
    FEEDS S-108 1
    PRODUCTS S-204 1 L / S-203 2 L / S-202 3 L / S-201  &
        4
    COMPR-SPECS 1 PRATIO=2.465032536 SEFF=0.8 / 2  &
        PRATIO=2.465032536 SEFF=0.8 / 3 PRATIO=2.465032536  &
        SEFF=0.8 / 4 PRATIO=2.465032536 SEFF=0.8
    COOLER-SPECS 1 TEMP=104.0000000 PDROP=10.00000000 / 2  &
        TEMP=104.0000000 PDROP=10.00000000 / 3 TEMP=104.0000000  &
        PDROP=10.00000000 / 4 TEMP=104.0000000 PDROP=10.00000000
```

```
BLOCK PR-201, VALVE
    PARAM P-OUT=200.0000000

BLOCK V-201 VALVE
    PARAM P-OUT=100.

BLOCK V-202 VALVE
    PARAM P-OUT=100.

BLOCK V-203 VALVE
    PARAM P-OUT=100.

DESIGN-SPEC BTXFLOW
    DEFINE BTXOUT STREAM-VAR STREAM=S-315 SUBSTREAM=MIXED  &
        VARIABLE=MASS-FLOW UOM="MMtons/year"
    SPEC "BTXOUT" TO "0.5"
    TOL-SPEC "0.01"
    VARY STREAM-VAR STREAM=S-101 SUBSTREAM=MIXED  &
        VARIABLE=MASS-FLOW UOM="MMtons/year"
    LIMITS "0" "100000"

DESIGN-SPEC CH4SPLIT
    DEFINE FURNQ BLOCK-VAR BLOCK=F-101 VARIABLE=NET-DUTY  &
        SENTENCE=RESULTS UOM="cal/sec"
    DEFINE HEATQ BLOCK-VAR BLOCK=F-101, VARIABLE=NET-DUTY  &
        SENTENCE=RESULTS UOM="cal/sec"
    DEFINE REACTQ BLOCK-VAR BLOCK=R-101 VARIABLE=NET-DUTY  &
        SENTENCE=RESULTS UOM="cal/sec"
    SPEC "FURNQ" TO "-(HEATQ+REACTQ)"
    TOL-SPEC "0.1"
    VARY BLOCK-VAR BLOCK=V-206 SENTENCE=FRAC VARIABLE=FRAC  &
        ID1=S-221
    LIMITS "0" "1"

DESIGN-SPEC SEP1PUR
    DEFINE BENBOT MASS-FLOW STREAM=S-310 SUBSTREAM=MIXED  &
        COMPONENT=BENZENE UOM="kg/hr"
    DEFINE BENFEED MASS-FLOW STREAM=S-210 SUBSTREAM=MIXED  &
        COMPONENT=BENZENE UOM="kg/hr"
    SPEC "BENBOT/BENFEED" TO "0.9"
    TOL-SPEC "0.01"
    VARY BLOCK-VAR BLOCK=COL-301 VARIABLE=MASS-D:F  &
        SENTENCE=COL-SPECS
    LIMITS "0" "1"

DESIGN-SPEC STEAMAMT
    DEFINE VAPFRAC STREAM-VAR STREAM=S-403 SUBSTREAM=MIXED  &
        VARIABLE=VFRAC
    SPEC "VAPFRAC" TO "1"
    TOL-SPEC "0.1"
    VARY STREAM-VAR STREAM=S-401 SUBSTREAM=MIXED  &
        VARIABLE=MASS-FLOW UOM="kg/hr"
    LIMITS "0" "6000000"

DESIGN-SPEC STEAMT
    DEFINE STEAMT STREAM-VAR STREAM=S-404 SUBSTREAM=MIXED  &
        VARIABLE=TEMP UOM="F"
```

```
    SPEC "STEAMT" TO "465"
    TOL-SPEC "1"
    VARY STREAM-VAR STREAM=S-401 SUBSTREAM=MIXED  &
        VARIABLE=MASS-FLOW UOM="kg/hr"
    LIMITS "400000" "500000"

DESIGN-SPEC STM1SPL
    DEFINE STM1TOUT STREAM-VAR STREAM=S-308 SUBSTREAM=MIXED  &
        VARIABLE=VFRAC
    SPEC "STM1TOUT" TO "0.05"
    TOL-SPEC "0.01"
    VARY BLOCK-VAR BLOCK=V-406-7 SENTENCE=FRAC VARIABLE=FRAC  &
        ID1=S-408
    LIMITS "0.30" "0.40"

DESIGN-SPEC STM2SPL
    DEFINE STM2TOUT STREAM-VAR STREAM=S-319 SUBSTREAM=MIXED  &
        VARIABLE=VFRAC
    SPEC "STM2TOUT" TO "0.05"
    TOL-SPEC "0.01"
    VARY BLOCK-VAR BLOCK=V-406-7 SENTENCE=FRAC VARIABLE=FRAC  &
        ID1=S-409
    LIMITS "0.35" "0.5"

DESIGN-SPEC STM3SPL
    DEFINE STM3TOUT STREAM-VAR STREAM=S-217 SUBSTREAM=MIXED  &
        VARIABLE=VFRAC
    SPEC "STM3TOUT" TO "0.05"
    TOL-SPEC "0.01"
    VARY BLOCK-VAR BLOCK=V-405 SENTENCE=FRAC VARIABLE=FRAC  &
        ID1=S-406
    LIMITS "0.05" "0.1"

EO-CONV-OPTI

CALCULATOR FURN1AIR
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar'
    DEFINE XCH4 MOLE-FRAC STREAM=S-220 SUBSTREAM=MIXED  &
        COMPONENT=METHANE
    DEFINE XC2H6 MOLE-FRAC STREAM=S-220 SUBSTREAM=MIXED  &
        COMPONENT=ETHANE
    DEFINE XC3H8 MOLE-FRAC STREAM=S-220 SUBSTREAM=MIXED  &
        COMPONENT=PROPANE
    DEFINE XH2 MOLE-FRAC STREAM=S-220 SUBSTREAM=MIXED  &
        COMPONENT=HYDROGEN
    DEFINE AIRREQ STREAM-VAR STREAM=S-109 SUBSTREAM=MIXED  &
        VARIABLE=MOLE-FLOW UOM="kmol/hr"
    DEFINE XO2 MOLE-FRAC STREAM=S-109 SUBSTREAM=MIXED  &
        COMPONENT=OXYGEN
    DEFINE FUELFLO STREAM-VAR STREAM=S-220 SUBSTREAM=MIXED  &
        VARIABLE=MOLE-FLOW UOM="kmol/hr"
F      AIRREQ = 1.2*FUELFLO*(2*XCH4+XH2/2)/XO2
    READ-VARS XCH4 XC2H6 XC3H8 XO2 FUELFLO XH2
    WRITE-VARS AIRREQ
    EXECUTE BEFORE BLOCK V-103
```

```
CALCULATOR FURN2AIR
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar'
    DEFINE AIRREQ STREAM-VAR STREAM=S-410 SUBSTREAM=MIXED  &
        VARIABLE=MOLE-FLOW UOM="kmol/hr"
    DEFINE H2FLOW MOLE-FLOW STREAM=S-221 SUBSTREAM=MIXED  &
        COMPONENT=HYDROGEN UOM="kmol/hr"
    DEFINE CH4FLOW MOLE-FLOW STREAM=S-221 SUBSTREAM=MIXED  &
        COMPONENT=METHANE UOM="kmol/hr"
F           AIRREQ = 1.2*(2*CH4FLOW+H2FLOW/2)/0.21
    READ-VARS H2FLOW CH4FLOW
    WRITE-VARS AIRREQ
    EXECUTE AFTER BLOCK V-206

CALCULATOR PUMPS
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar'
    DEFINE PUMP1P BLOCK-VAR BLOCK=P-201 VARIABLE=PRES  &
        SENTENCE=PARAM UOM="bar"
    DEFINE VALVE2P BLOCK-VAR BLOCK=V-203 VARIABLE=P-OUT  &
        SENTENCE=PARAM UOM="bar"
    DEFINE VALVE3P BLOCK-VAR BLOCK=V-202 VARIABLE=P-OUT  &
        SENTENCE=PARAM UOM="bar"
    DEFINE VALVE4P BLOCK-VAR BLOCK=V-201 VARIABLE=P-OUT  &
        SENTENCE=PARAM UOM="bar"
    DEFINE COLP BLOCK-VAR BLOCK=COL-301 VARIABLE=PRES  &
        SENTENCE=PROFILE ID1=14 UOM="bar"
F     PUMP1P = COLP
F     VALVE2P = COLP
F     VALVE3P = COLP
F     VALVE4P = COLP
    READ-VARS COLP
    WRITE-VARS PUMP1P VALVE2P VALVE3P VALVE4P
    EXECUTE AFTER BLOCK COL-301

CONV-OPTIONS
    PARAM TEAR-METHOD=WEGSTEIN TOL=0.0001 SPEC-METHOD=SECANT

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

DISABLE
    CALCULATOR PUMPS
    DESIGN-SPEC STEAMAMT
```

### *A-5.2. Stream Report*

HEAT1 HEAT2 HEAT3 HEAT4

| STREAM ID | | HEAT1 | HEAT2 | HEAT3 | HEAT4 |
|---|---|---|---|---|---|
| FROM : | | F-401-2 | H-203 | COL-301 | COL-302 |
| TO : | | F-401-2, | H-203, | RB-301 | RB-302 |
| CLASS: | | HEAT | HEAT | HEAT | HEAT |
| STREAM ATTRIBUTES: | | | | | |
| HEAT | | | | | |
| Q | BTU/HR | 1.3050+09 | -1.5007+07 | -9.0323+06 | -2.8999+07 |
| TBEG | F | 94.7830 | 129.6288 | 195.7211 | 323.0151 |
| TEND | F | 572.0000 | 181.4000 | 200.4235 | 323.7883 |

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

| STREAM ID | S-101 | S-102 | S-103 | S-104 | S-105 |
|---|---|---|---|---|---|
| FROM : | ---- | T-102 | T-101 | T-103 | V-101-2 |
| TO : | T-102 | V-101-2 | V-101-2 | V-101-2 | H-101 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | VAPOR | MIXED | MIXED | MIXED |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 1394.8100 | 5.2075-05 | 1394.8100 |
| METHANE | 62.8392 | 62.8392 | 7314.0134 | 172.6175 | 7549.4701 |
| ETHANE | 6095.4040 | 6095.4040 | 6865.2255 | 238.5242 | 1.3199+04 |
| ETHENE | 0.0 | 0.0 | 780.6162 | 22.0910 | 802.7072 |
| PROPANE | 125.6784 | 125.6784 | 192.2615 | 16.4274 | 334.3674 |
| PROPENE | 0.0 | 0.0 | 63.7247 | 3.4654 | 67.1900 |
| BENZENE | 0.0 | 0.0 | 125.7796 | 108.5439 | 234.3235 |
| TOLUENE | 0.0 | 0.0 | 4.4111 | 10.4562 | 14.8673 |
| P-XYL-01 | 0.0 | 0.0 | 3.5762-02 | 0.1014 | 0.1372 |
| 1:3:5-01 | 0.0 | 0.0 | 9.2656-04 | 1.8392-07 | 9.2675-04 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 8.3318-02 | 9.1005-08 | 5.9110-02 |
| METHANE | 1.0000-02 | 1.0000-02 | 0.4369 | 0.3017 | 0.3199 |
| ETHANE | 0.9700 | 0.9700 | 0.4101 | 0.4168 | 0.5594 |
| ETHENE | 0.0 | 0.0 | 4.6629-02 | 3.8605-02 | 3.4017-02 |
| PROPANE | 2.0000-02 | 2.0000-02 | 1.1485-02 | 2.8708-02 | 1.4170-02 |
| PROPENE | 0.0 | 0.0 | 3.8065-03 | 6.0559-03 | 2.8474-03 |
| BENZENE | 0.0 | 0.0 | 7.5133-03 | 0.1897 | 9.9302-03 |
| TOLUENE | 0.0 | 0.0 | 2.6350-04 | 1.8273-02 | 6.3005-04 |
| P-XYL-01 | 0.0 | 0.0 | 2.1362-06 | 1.7728-04 | 5.8146-06 |
| 1:3:5-01 | 0.0 | 0.0 | 5.5347-08 | 3.2141-10 | 3.9274-08 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 2811.7695 | 1.0498-04 | 2811.7696 |
| METHANE | 1008.1145 | 1008.1145 | 1.1734+05 | 2769.2615 | 1.2111+05 |
| ETHANE | 1.8329+05 | 1.8329+05 | 2.0643+05 | 7172.3375 | 3.9689+05 |
| ETHENE | 0.0 | 0.0 | 2.1899+04 | 619.7359 | 2.2519+04 |
| PROPANE | 5541.9815 | 5541.9815 | 8478.0651 | 724.3933 | 1.4744+04 |
| PROPENE | 0.0 | 0.0 | 2681.5743 | 145.8246 | 2827.3989 |
| BENZENE | 0.0 | 0.0 | 9825.0998 | 8478.7610 | 1.8304+04 |
| TOLUENE | 0.0 | 0.0 | 406.4449 | 963.4368 | 1369.8817 |
| P-XYL-01 | 0.0 | 0.0 | 3.7968 | 10.7700 | 14.5668 |
| 1:3:5-01 | 0.0 | 0.0 | 0.1114 | 2.2106-05 | 0.1114 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 7.6019-03 | 5.0266-09 | 4.8429-03 |
| METHANE | 5.3104-03 | 5.3104-03 | 0.3172 | 0.1326 | 0.2086 |
| ETHANE | 0.9655 | 0.9655 | 0.5581 | 0.3434 | 0.6836 |
| ETHENE | 0.0 | 0.0 | 5.9207-02 | 2.9674-02 | 3.8786-02 |
| PROPANE | 2.9193-02 | 2.9193-02 | 2.2921-02 | 3.4686-02 | 2.5395-02 |
| PROPENE | 0.0 | 0.0 | 7.2499-03 | 6.9824-03 | 4.8698-03 |
| BENZENE | 0.0 | 0.0 | 2.6563-02 | 0.4060 | 3.1526-02 |
| TOLUENE | 0.0 | 0.0 | 1.0989-03 | 4.6132-02 | 2.3594-03 |
| P-XYL-01 | 0.0 | 0.0 | 1.0265-05 | 5.1570-04 | 2.5089-05 |
| 1:3:5-01 | 0.0 | 0.0 | 3.0109-07 | 1.0585-09 | 1.9185-07 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 6283.9216 | 6283.9216 | 1.6741+04 | 572.2272 | 2.3597+04 |
| LB/HR | 1.8984+05 | 1.8984+05 | 3.6988+05 | 2.0885+04 | 5.8060+05 |
| CUFT/HR | 1.1683+05 | 5.0021+05 | 1.3984+06 | 6.9614+04 | 1.9998+06 |
| STATE VARIABLES: | | | | | |
| TEMP F | 80.0000 | -37.4871 | -26.9538 | 166.6616 | -17.0838 |
| PRES PSIA | 264.6959 | 53.6640 | 53.6640 | 53.6640 | 53.6640 |
| VFRAC | 1.0000 | 1.0000 | 0.9908 | 0.9943 | 0.9874 |
| LFRAC | 0.0 | 0.0 | 9.1642-03 | 5.6769-03 | 1.2647-02 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -3.6611+04 | -3.7670+04 | -2.9149+04 | -1.6819+04 | -3.1119+04 |
| BTU/LB | -1211.8994 | -1246.9321 | -1319.2949 | -460.8216 | -1264.7549 |
| BTU/HR | -2.3006+08 | -2.3671+08 | -4.8798+08 | -9.6240+06 | -7.3432+08 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -47.7691 | -47.1251 | -29.9197 | -31.7680 | -34.1442 |
| BTU/LB-R | -1.5812 | -1.5599 | -1.3542 | -0.8704 | -1.3877 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 5.3787-02 | 1.2563-02 | 1.1971-02 | 8.2200-03 | 1.1800-02 |
| LB/CUFT | 1.6249 | 0.3795 | 0.2645 | 0.3000 | 0.2903 |
| AVG MW | 30.2099 | 30.2099 | 22.0943 | 36.4969 | 24.6048 |

S-106 S-106, S-107 S-108 S-109
------------------------------

| STREAM ID | S-106 | S-106, | S-107 | S-108 | S-109 |
|---|---|---|---|---|---|
| FROM : | H-101 | F-101, | R-101 | H-101 | ---- |

| TO : | F-101, | R-101 | H-101 | C-201-3 | V-103 |
|---|---|---|---|---|---|
| MAX CONV. ERROR: | -1.4695-05 | 0.0 | 0.0 | 0.0 | 0.0 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | VAPOR | VAPOR | MIXED | VAPOR |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 1394.8100 | 1394.8101 | 9298.7333 | 9298.7333 | 0.0 |
| METHANE | 7549.4701 | 7549.5749 | 1.0331+04 | 1.0331+04 | 0.0 |
| ETHANE | 1.3199+04 | 1.3199+04 | 7103.7498 | 7103.7498 | 0.0 |
| ETHENE | 802.7072 | 802.7072 | 802.7072 | 802.7072 | 0.0 |
| PROPANE | 334.3674 | 334.3674 | 208.6890 | 208.6890 | 0.0 |
| PROPENE | 67.1900 | 67.1900 | 67.1900 | 67.1900 | 0.0 |
| BENZENE | 234.3235 | 234.3241 | 1151.3585 | 1151.3585 | 0.0 |
| TOLUENE | 14.8673 | 14.8673 | 398.4794 | 398.4794 | 0.0 |
| P-XYL-01 | 0.1372 | 0.1372 | 88.0037 | 88.0037 | 0.0 |
| 1:3:5-01 | 9.2675-04 | 9.2676-04 | 99.5612 | 99.5612 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 2032.4726 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 7645.9682 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 5.9110-02 | 5.9109-02 | 0.3147 | 0.3147 | 0.0 |
| METHANE | 0.3199 | 0.3199 | 0.3496 | 0.3496 | 0.0 |
| ETHANE | 0.5594 | 0.5594 | 0.2404 | 0.2404 | 0.0 |
| ETHENE | 3.4017-02 | 3.4017-02 | 2.7165-02 | 2.7165-02 | 0.0 |
| PROPANE | 1.4170-02 | 1.4170-02 | 7.0624-03 | 7.0624-03 | 0.0 |
| PROPENE | 2.8474-03 | 2.8474-03 | 2.2738-03 | 2.2738-03 | 0.0 |
| BENZENE | 9.9302-03 | 9.9302-03 | 3.8964-02 | 3.8964-02 | 0.0 |
| TOLUENE | 6.3005-04 | 6.3005-04 | 1.3485-02 | 1.3485-02 | 0.0 |
| P-XYL-01 | 5.8146-06 | 5.8145-06 | 2.9782-03 | 2.9782-03 | 0.0 |
| 1:3:5-01 | 3.9274-08 | 3.9274-08 | 3.3693-03 | 3.3693-03 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.2100 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.7900 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 2811.7696 | 2811.7697 | 1.8745+04 | 1.8745+04 | 0.0 |
| METHANE | 1.2111+05 | 1.2112+05 | 1.6574+05 | 1.6574+05 | 0.0 |
| ETHANE | 3.9689+05 | 3.9689+05 | 2.1361+05 | 2.1361+05 | 0.0 |
| ETHENE | 2.2519+04 | 2.2519+04 | 2.2519+04 | 2.2519+04 | 0.0 |
| PROPANE | 1.4744+04 | 1.4744+04 | 9202.4586 | 9202.4586 | 0.0 |
| PROPENE | 2827.3989 | 2827.3990 | 2827.3990 | 2827.3990 | 0.0 |
| BENZENE | 1.8304+04 | 1.8304+04 | 8.9937+04 | 8.9937+04 | 0.0 |
| TOLUENE | 1369.8817 | 1369.8824 | 3.6716+04 | 3.6716+04 | 0.0 |
| P-XYL-01 | 14.5668 | 14.5667 | 9343.1188 | 9343.1188 | 0.0 |
| 1:3:5-01 | 0.1114 | 0.1114 | 1.1967+04 | 1.1967+04 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 6.5037+04 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 2.1419+05 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 4.8429-03 | 4.8429-03 | 3.2286-02 | 3.2286-02 | 0.0 |
| METHANE | 0.2086 | 0.2086 | 0.2855 | 0.2855 | 0.0 |
| ETHANE | 0.6836 | 0.6836 | 0.3679 | 0.3679 | 0.0 |
| ETHENE | 3.8786-02 | 3.8786-02 | 3.8786-02 | 3.8786-02 | 0.0 |
| PROPANE | 2.5395-02 | 2.5395-02 | 1.5850-02 | 1.5850-02 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| PROPENE | 4.8698-03 | 4.8698-03 | 4.8698-03 | 4.8698-03 | 0.0 |
| BENZENE | 3.1526-02 | 3.1526-02 | 0.1549 | 0.1549 | 0.0 |
| TOLUENE | 2.3594-03 | 2.3594-03 | 6.3238-02 | 6.3238-02 | 0.0 |
| P-XYL-01 | 2.5089-05 | 2.5089-05 | 1.6092-02 | 1.6092-02 | 0.0 |
| 1:3:5-01 | 1.9185-07 | 1.9186-07 | 2.0611-02 | 2.0611-02 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.2329 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.7671 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 2.3597+04 | 2.3597+04 | 2.9549+04 | 2.9549+04 | 9678.4408 |
| LB/HR | 5.8060+05 | 5.8060+05 | 5.8060+05 | 5.8060+05 | 2.7923+05 |
| CUFT/HR | 9.3271+06 | 9.4317+06 | 1.4165+07 | 6.6808+06 | 3.8414+06 |
| STATE VARIABLES: | | | | | |
| TEMP F | 1148.0000 | 1166.0000 | 1166.0000 | 102.9178 | 77.0000 |
| PRES PSIA | 43.6640 | 43.6640 | 36.4121 | 26.4121 | 14.5038 |
| VFRAC | 1.0000 | 1.0000 | 1.0000 | 0.9928 | 1.0000 |
| LFRAC | 0.0 | 0.0 | 0.0 | 7.2463-03 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -1.1199+04 | -1.0785+04 | -1836.7363 | -1.7744+04 | -2.8903 |
| BTU/LB | -455.1462 | -438.3481 | -93.4799 | -903.0861 | -0.1002 |
| BTU/HR | -2.6426+08 | -2.5451+08 | -5.4275+07 | -5.2433+08 | -2.7974+04 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -13.3095 | -13.0538 | -3.9814 | -18.5047 | 1.0423 |
| BTU/LB-R | -0.5409 | -0.5305 | -0.2026 | -0.9418 | 3.6128-02 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 2.5299-03 | 2.5019-03 | 2.0861-03 | 4.4230-03 | 2.5195-03 |
| LB/CUFT | 6.2249-02 | 6.1558-02 | 4.0988-02 | 8.6905-02 | 7.2689-02 |
| AVG MW | 24.6048 | 24.6047 | 19.6485 | 19.6485 | 28.8504 |

S-110 S-201 S-202 S-203 S-204
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| STREAM ID | S-110 | S-201 | S-202 | S-203 | S-204 |
|---|---|---|---|---|---|
| FROM : | F-101 | C-201-3 | C-201-3 | C-201-3 | C-201-3 |
| TO : | ---- | COL-201 | V-202 | V-203 | P-201 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | MIXED | LIQUID | LIQUID | LIQUID |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 9298.7333 | 1.4112-05 | 6.6093-06 | 3.9946-06 |
| METHANE | 0.0 | 1.0241+04 | 49.7312 | 24.8481 | 15.4312 |
| ETHANE | 0.0 | 6968.5278 | 72.2086 | 38.4651 | 24.5482 |
| ETHENE | 0.0 | 790.4191 | 6.6169 | 3.4709 | 2.2003 |
| PROPANE | 0.0 | 199.1530 | 5.0230 | 2.7416 | 1.7713 |
| PROPENE | 0.0 | 65.2797 | 0.9903 | 0.5385 | 0.3815 |
| BENZENE | 0.0 | 273.1375 | 267.8718 | 300.5154 | 309.8338 |
| TOLUENE | 0.0 | 18.3614 | 52.3147 | 117.4845 | 210.3187 |
| P-XYL-01 | 0.0 | 0.3389 | 2.8720 | 16.5359 | 68.2569 |
| 1:3:5-01 | 0.0 | 2.1683-02 | 0.5189 | 8.1958 | 90.8248 |
| WATER | 2388.0322 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 338.7454 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 7645.9682 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 499.7110 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.3338 | 3.0803-08 | 1.2889-08 | 5.5207-09 |

| | | | | | |
|---|---|---|---|---|---|
| METHANE | 0.0 | 0.3677 | 0.1085 | 4.8456-02 | 2.1327-02 |
| ETHANE | 0.0 | 0.2502 | 0.1576 | 7.5011-02 | 3.3927-02 |
| ETHENE | 0.0 | 2.8376-02 | 1.4443-02 | 6.7685-03 | 3.0409-03 |
| PROPANE | 0.0 | 7.1497-03 | 1.0964-02 | 5.3464-03 | 2.4481-03 |
| PROPENE | 0.0 | 2.3436-03 | 2.1616-03 | 1.0501-03 | 5.2728-04 |
| BENZENE | 0.0 | 9.8057-03 | 0.5847 | 0.5860 | 0.4282 |
| TOLUENE | 0.0 | 6.5918-04 | 0.1142 | 0.2291 | 0.2907 |
| P-XYL-01 | 0.0 | 1.2166-05 | 6.2686-03 | 3.2247-02 | 9.4334-02 |
| 1:3:5-01 | 0.0 | 7.7842-07 | 1.1325-03 | 1.5983-02 | 0.1255 |
| WATER | 0.2196 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 3.1156-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.7032 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 4.5961-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 1.8745+04 | 2.8448-05 | 1.3323-05 | 8.0526-06 |
| METHANE | 0.0 | 1.6429+05 | 797.8258 | 398.6320 | 247.5598 |
| ETHANE | 0.0 | 2.0954+05 | 2171.2867 | 1156.6322 | 738.1570 |
| ETHENE | 0.0 | 2.2174+04 | 185.6288 | 97.3707 | 61.7273 |
| PROPANE | 0.0 | 8781.9546 | 221.4973 | 120.8966 | 78.1101 |
| PROPENE | 0.0 | 2747.0108 | 41.6738 | 22.6597 | 16.0546 |
| BENZENE | 0.0 | 2.1336+04 | 2.0924+04 | 2.3474+04 | 2.4202+04 |
| TOLUENE | 0.0 | 1691.8323 | 4820.3074 | 1.0825+04 | 1.9379+04 |
| P-XYL-01 | 0.0 | 35.9784 | 304.9079 | 1755.5779 | 7246.6547 |
| 1:3:5-01 | 0.0 | 2.6062 | 62.3656 | 985.0911 | 1.0917+04 |
| WATER | 4.3021+04 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 1.0839+04 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 2.1419+05 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 2.1992+04 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 4.1716-02 | 9.6337-10 | 3.4307-10 | 1.2805-10 |
| METHANE | 0.0 | 0.3656 | 2.7018-02 | 1.0264-02 | 3.9366-03 |
| ETHANE | 0.0 | 0.4663 | 7.3528-02 | 2.9782-02 | 1.1738-02 |
| ETHENE | 0.0 | 4.9347-02 | 6.2861-03 | 2.5072-03 | 9.8157-04 |
| PROPANE | 0.0 | 1.9544-02 | 7.5008-03 | 3.1130-03 | 1.2421-03 |
| PROPENE | 0.0 | 6.1133-03 | 1.4112-03 | 5.8347-04 | 2.5530-04 |
| BENZENE | 0.0 | 4.7482-02 | 0.7086 | 0.6044 | 0.3849 |
| TOLUENE | 0.0 | 3.7651-03 | 0.1632 | 0.2787 | 0.3082 |
| P-XYL-01 | 0.0 | 8.0068-05 | 1.0325-02 | 4.5205-02 | 0.1152 |
| 1:3:5-01 | 0.0 | 5.7999-06 | 2.1119-03 | 2.5365-02 | 0.1736 |
| WATER | 0.1483 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 3.7372-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.7385 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 7.5824-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 1.0872+04 | 2.7855+04 | 458.1474 | 512.7958 | 723.5669 |
| LB/HR | 2.9004+05 | 4.4935+05 | 2.9530+04 | 3.8836+04 | 6.2886+04 |
| CUFT/HR | 1.4528+07 | 2.1502+05 | 628.3836 | 769.1817 | 1215.1836 |
| STATE VARIABLES: | | | | | |
| TEMP F | 1346.0000 | 104.0000 | 104.0000 | 104.0000 | 104.0000 |
| PRES PSIA | 14.5038 | 729.9998 | 300.1988 | 125.8396 | 55.1066 |
| VFRAC | 1.0000 | 0.9869 | 0.0 | 0.0 | 0.0 |
| LFRAC | 0.0 | 1.3132-02 | 1.0000 | 1.0000 | 1.0000 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -2.0655+04 | -2.0222+04 | 3386.3202 | 8841.0617 | 4917.6703 |
| BTU/LB | -774.2822 | -1253.5260 | 52.5377 | 116.7377 | 56.5828 |
| BTU/HR | -2.2458+08 | -5.6327+08 | 1.5514+06 | 4.5337+06 | 3.5583+06 |

| | | | | | |
|---|---|---|---|---|---|
| ENTROPY: | | | | | |
| BTU/LBMOL-R | 8.7412 | -24.0792 | -55.0192 | -62.0678 | -74.9013 |
| BTU/LB-R | 0.3277 | -1.4927 | -0.8536 | -0.8195 | -0.8618 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 7.4838-04 | 0.1295 | 0.7291 | 0.6667 | 0.5954 |
| LB/CUFT | 1.9964-02 | 2.0898 | 46.9935 | 50.4904 | 51.7502 |
| AVG MW | 26.6768 | 16.1318 | 64.4551 | 75.7344 | 86.9111 |

S-205 S-206 S-207 S-208 S-209
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| STREAM ID | S-205 | S-206 | S-207 | S-208 | S-209 |
|---|---|---|---|---|---|
| FROM : | COL-201 | V-201 | V-202 | V-203 | P-201 |
| TO : | V-201 | V-203-5 | V-203-5 | V-203-5 | V-203-5 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | LIQUID | MIXED | MIXED | MIXED | LIQUID |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 2.7359-05 | 2.7359-05 | 1.4112-05 | 6.6093-06 | 3.9946-06 |
| METHANE | 82.6084 | 82.6084 | 49.7312 | 24.8481 | 15.4312 |
| ETHANE | 103.3017 | 103.3017 | 72.2086 | 38.4651 | 24.5482 |
| ETHENE | 9.8029 | 9.8029 | 6.6169 | 3.4709 | 2.2003 |
| PROPANE | 6.8914 | 6.8914 | 5.0230 | 2.7416 | 1.7713 |
| PROPENE | 1.5550 | 1.5550 | 0.9903 | 0.5385 | 0.3815 |
| BENZENE | 147.3575 | 147.3575 | 267.8718 | 300.5154 | 309.8338 |
| TOLUENE | 13.9503 | 13.9503 | 52.3147 | 117.4845 | 210.3187 |
| P-XYL-01 | 0.3031 | 0.3031 | 2.8720 | 16.5359 | 68.2569 |
| 1:3:5-01 | 2.0756-02 | 2.0756-02 | 0.5189 | 8.1958 | 90.8248 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 7.4795-08 | 7.4795-08 | 3.0803-08 | 1.2889-08 | 5.5207-09 |
| METHANE | 0.2258 | 0.2258 | 0.1085 | 4.8456-02 | 2.1327-02 |
| ETHANE | 0.2824 | 0.2824 | 0.1576 | 7.5011-02 | 3.3927-02 |
| ETHENE | 2.6799-02 | 2.6799-02 | 1.4443-02 | 6.7685-03 | 3.0409-03 |
| PROPANE | 1.8840-02 | 1.8840-02 | 1.0964-02 | 5.3464-03 | 2.4481-03 |
| PROPENE | 4.2511-03 | 4.2511-03 | 2.1616-03 | 1.0501-03 | 5.2728-04 |
| BENZENE | 0.4028 | 0.4028 | 0.5847 | 0.5860 | 0.4282 |
| TOLUENE | 3.8137-02 | 3.8137-02 | 0.1142 | 0.2291 | 0.2907 |
| P-XYL-01 | 8.2867-04 | 8.2867-04 | 6.2686-03 | 3.2247-02 | 9.4334-02 |
| 1:3:5-01 | 5.6744-05 | 5.6744-05 | 1.1325-03 | 1.5983-02 | 0.1255 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 5.5153-05 | 5.5153-05 | 2.8448-05 | 1.3323-05 | 8.0526-06 |
| METHANE | 1325.2672 | 1325.2672 | 797.8258 | 398.6320 | 247.5598 |
| ETHANE | 3106.2458 | 3106.2458 | 2171.2867 | 1156.6322 | 738.1570 |
| ETHENE | 275.0077 | 275.0077 | 185.6288 | 97.3707 | 61.7273 |
| PROPANE | 303.8877 | 303.8877 | 221.4973 | 120.8966 | 78.1101 |
| PROPENE | 65.4362 | 65.4362 | 41.6738 | 22.6597 | 16.0546 |
| BENZENE | 1.1511+04 | 1.1511+04 | 2.0924+04 | 2.3474+04 | 2.4202+04 |
| TOLUENE | 1285.3839 | 1285.3839 | 4820.3074 | 1.0825+04 | 1.9379+04 |
| P-XYL-01 | 32.1816 | 32.1816 | 304.9079 | 1755.5779 | 7246.6547 |

```
  1:3:5-01              2.4948      2.4948     62.3656    985.0911  1.0917+04
  WATER                 0.0         0.0         0.0         0.0         0.0
  OXYGEN                0.0         0.0         0.0         0.0         0.0
  NITROGEN              0.0         0.0         0.0         0.0         0.0
  CARBO-01              0.0         0.0         0.0         0.0         0.0
COMPONENTS: MASS FRAC
  HYDROGEN           3.0801-09   3.0801-09   9.6337-10   3.4307-10   1.2805-10
  METHANE            7.4010-02   7.4010-02   2.7018-02   1.0264-02   3.9366-03
  ETHANE                0.1735      0.1735   7.3528-02   2.9782-02   1.1738-02
  ETHENE             1.5358-02   1.5358-02   6.2861-03   2.5072-03   9.8157-04
  PROPANE            1.6971-02   1.6971-02   7.5008-03   3.1130-03   1.2421-03
  PROPENE            3.6543-03   3.6543-03   1.4112-03   5.8347-04   2.5530-04
  BENZENE               0.6428      0.6428      0.7086      0.6044      0.3849
  TOLUENE            7.1783-02   7.1783-02      0.1632      0.2787      0.3082
  P-XYL-01           1.7972-03   1.7972-03   1.0325-02   4.5205-02      0.1152
  1:3:5-01           1.3932-04   1.3932-04   2.1119-03   2.5365-02      0.1736
  WATER                 0.0         0.0         0.0         0.0         0.0
  OXYGEN                0.0         0.0         0.0         0.0         0.0
  NITROGEN              0.0         0.0         0.0         0.0         0.0
  CARBO-01              0.0         0.0         0.0         0.0         0.0
TOTAL FLOW:
  LBMOL/HR            365.7911    365.7911    458.1474    512.7958    723.5669
  LB/HR              1.7907+04   1.7907+04   2.9530+04   3.8836+04   6.2886+04
  CUFT/HR             456.9599   8.8319+04   6.5919+04   3.5235+04   1215.1168
STATE VARIABLES:
  TEMP   F            104.0000     20.7594     63.1154     85.5026    103.9130
  PRES   PSIA         729.9998     11.8000     11.8000     11.8000     11.8000
  VFRAC                 0.0         0.5545      0.3023      0.1368      0.0
  LFRAC                 1.0000      0.4455      0.6977      0.8632      1.0000
  SFRAC                 0.0         0.0         0.0         0.0         0.0
ENTHALPY:
  BTU/LBMOL         -9995.5132  -9995.5132   3386.3202   8841.0617   4906.9032
  BTU/LB             -204.1864   -204.1864     52.5377    116.7377     56.4589
  BTU/HR            -3.6563+06  -3.6563+06   1.5514+06   4.5337+06   3.5505+06
ENTROPY:
  BTU/LBMOL-R         -48.8363    -45.6916    -53.7914    -61.6982    -74.8959
  BTU/LB-R             -0.9976     -0.9334     -0.8346     -0.8147     -0.8618
DENSITY:
  LBMOL/CUFT            0.8005   4.1417-03   6.9502-03   1.4554-02      0.5955
  LB/CUFT              39.1862      0.2027      0.4480      1.1022     51.7531
AVG MW                 48.9529     48.9529     64.4551     75.7344     86.9111

S-210 S-211 S-212 S-213 S-214
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STREAM ID              S-210       S-211       S-212       S-213       S-214
FROM :                 V-203-5     COL-201     H-201       H-202       H-203
TO   :                 COL-301     H-201       H-202       H-203       PR-201


MAX CONV. ERROR:    -1.2179-05   1.0193-05      0.0         0.0         0.0
SUBSTREAM: MIXED
PHASE:                 MIXED       VAPOR       VAPOR       VAPOR       VAPOR
COMPONENTS: LBMOL/HR
  HYDROGEN           5.2075-05   9298.7332   9298.7332   9298.7332   9298.7332
  METHANE             172.6175   1.0158+04   1.0158+04   1.0158+04   1.0158+04
  ETHANE              238.5243   6865.2255   6865.2255   6865.2255   6865.2255
```

| | | | | | |
|---|---|---|---|---|---|
| ETHENE | 22.0910 | 780.6162 | 780.6162 | 780.6162 | 780.6162 |
| PROPANE | 16.4274 | 192.2615 | 192.2615 | 192.2615 | 192.2615 |
| PROPENE | 3.4654 | 63.7247 | 63.7247 | 63.7247 | 63.7247 |
| BENZENE | 1025.5849 | 125.7796 | 125.7796 | 125.7796 | 125.7796 |
| TOLUENE | 394.0676 | 4.4111 | 4.4111 | 4.4111 | 4.4111 |
| P-XYL-01 | 87.9679 | 3.5762-02 | 3.5762-02 | 3.5762-02 | 3.5762-02 |
| 1:3:5-01 | 99.5603 | 9.2656-04 | 9.2656-04 | 9.2656-04 | 9.2656-04 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 2.5276-08 | 0.3383 | 0.3383 | 0.3383 | 0.3383 |
| METHANE | 8.3782-02 | 0.3695 | 0.3695 | 0.3695 | 0.3695 |
| ETHANE | 0.1158 | 0.2497 | 0.2497 | 0.2497 | 0.2497 |
| ETHENE | 1.0722-02 | 2.8397-02 | 2.8397-02 | 2.8397-02 | 2.8397-02 |
| PROPANE | 7.9733-03 | 6.9941-03 | 6.9941-03 | 6.9941-03 | 6.9941-03 |
| PROPENE | 1.6820-03 | 2.3182-03 | 2.3182-03 | 2.3182-03 | 2.3182-03 |
| BENZENE | 0.4978 | 4.5756-03 | 4.5756-03 | 4.5756-03 | 4.5756-03 |
| TOLUENE | 0.1913 | 1.6047-04 | 1.6047-04 | 1.6047-04 | 1.6047-04 |
| P-XYL-01 | 4.2697-02 | 1.3010-06 | 1.3010-06 | 1.3010-06 | 1.3010-06 |
| 1:3:5-01 | 4.8323-02 | 3.3706-08 | 3.3706-08 | 3.3706-08 | 3.3706-08 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 1.0498-04 | 1.8745+04 | 1.8745+04 | 1.8745+04 | 1.8745+04 |
| METHANE | 2769.2619 | 1.6297+05 | 1.6297+05 | 1.6297+05 | 1.6297+05 |
| ETHANE | 7172.3384 | 2.0643+05 | 2.0643+05 | 2.0643+05 | 2.0643+05 |
| ETHENE | 619.7360 | 2.1899+04 | 2.1899+04 | 2.1899+04 | 2.1899+04 |
| PROPANE | 724.3933 | 8478.0651 | 8478.0651 | 8478.0651 | 8478.0651 |
| PROPENE | 145.8246 | 2681.5743 | 2681.5743 | 2681.5743 | 2681.5743 |
| BENZENE | 8.0112+04 | 9825.0998 | 9825.0998 | 9825.0998 | 9825.0998 |
| TOLUENE | 3.6310+04 | 406.4449 | 406.4449 | 406.4449 | 406.4449 |
| P-XYL-01 | 9339.3203 | 3.7968 | 3.7968 | 3.7968 | 3.7968 |
| 1:3:5-01 | 1.1967+04 | 0.1114 | 0.1114 | 0.1114 | 0.1114 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 7.0380-10 | 4.3448-02 | 4.3448-02 | 4.3448-02 | 4.3448-02 |
| METHANE | 1.8566-02 | 0.3777 | 0.3777 | 0.3777 | 0.3777 |
| ETHANE | 4.8085-02 | 0.4785 | 0.4785 | 0.4785 | 0.4785 |
| ETHENE | 4.1549-03 | 5.0758-02 | 5.0758-02 | 5.0758-02 | 5.0758-02 |
| PROPANE | 4.8565-03 | 1.9651-02 | 1.9651-02 | 1.9651-02 | 1.9651-02 |
| PROPENE | 9.7764-04 | 6.2154-03 | 6.2154-03 | 6.2154-03 | 6.2154-03 |
| BENZENE | 0.5371 | 2.2773-02 | 2.2773-02 | 2.2773-02 | 2.2773-02 |
| TOLUENE | 0.2434 | 9.4206-04 | 9.4206-04 | 9.4206-04 | 9.4206-04 |
| P-XYL-01 | 6.2613-02 | 8.8002-06 | 8.8002-06 | 8.8002-06 | 8.8002-06 |
| 1:3:5-01 | 8.0227-02 | 2.5813-07 | 2.5813-07 | 2.5813-07 | 2.5813-07 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| LBMOL/HR | 2060.3064 | 2.7489+04 | 2.7489+04 | 2.7489+04 | 2.7489+04 |
| LB/HR | 1.4916+05 | 4.3144+05 | 4.3144+05 | 4.3144+05 | 4.3144+05 |
| CUFT/HR | 2.2662+05 | 2.1456+05 | 2.2845+05 | 2.3339+05 | 2.6174+05 |
| STATE VARIABLES: | | | | | |
| TEMP F | 75.8440 | 104.0000 | 126.3420 | 129.6288 | 181.4000 |
| PRES PSIA | 11.8000 | 729.9998 | 719.9998 | 709.9998 | 699.9998 |
| VFRAC | 0.2247 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| LFRAC | 0.7753 | 0.0 | 0.0 | 0.0 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | 2902.1834 | -2.0358+04 | -2.0122+04 | -2.0084+04 | -1.9538+04 |
| BTU/LB | 40.0873 | -1297.0781 | -1282.0629 | -1279.6658 | -1244.8834 |
| BTU/HR | 5.9794+06 | -5.5961+08 | -5.5314+08 | -5.5210+08 | -5.3710+08 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -61.5267 | -23.7498 | -23.3138 | -23.2234 | -22.3085 |
| BTU/LB-R | -0.8499 | -1.5132 | -1.4854 | -1.4797 | -1.4214 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 9.0916-03 | 0.1281 | 0.1203 | 0.1178 | 0.1050 |
| LB/CUFT | 0.6582 | 2.0108 | 1.8886 | 1.8486 | 1.6483 |
| AVG MW | 72.3966 | 15.6950 | 15.6950 | 15.6950 | 15.6950 |

S-215 S-216 S-217 S-218 S-219
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| STREAM ID | S-215 | S-216 | S-217 | S-218 | S-219 |
|---|---|---|---|---|---|
| FROM : | H-201 | H-202 | H-203, | PR-201 | PR-201, |
| TO : | ---- | ---- | V-401-3 | T-101 | V-206 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | LIQUID | LIQUID | MIXED | VAPOR | VAPOR |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 1394.8100 | 7903.9232 |
| METHANE | 0.0 | 0.0 | 0.0 | 7314.0134 | 2844.3385 |
| ETHANE | 0.0 | 0.0 | 0.0 | 6865.2255 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 780.6162 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 192.2615 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 63.7247 | 0.0 |
| BENZENE | 917.0410 | 4.8566-09 | 0.0 | 125.7796 | 0.0 |
| TOLUENE | 383.6114 | 1.8879-05 | 0.0 | 4.4111 | 0.0 |
| P-XYL-01 | 87.8297 | 3.6709-02 | 0.0 | 3.5762-02 | 0.0 |
| 1:3:5-01 | 0.2518 | 99.3085 | 0.0 | 9.2656-04 | 0.0 |
| WATER | 0.0 | 0.0 | 1073.4269 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 8.3318-02 | 0.7354 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.4369 | 0.2646 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.4101 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 4.6629-02 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 1.1485-02 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 3.8065-03 | 0.0 |
| BENZENE | 0.6603 | 4.8886-11 | 0.0 | 7.5133-03 | 0.0 |
| TOLUENE | 0.2762 | 1.9003-07 | 0.0 | 2.6350-04 | 0.0 |
| P-XYL-01 | 6.3244-02 | 3.6951-04 | 0.0 | 2.1362-06 | 0.0 |
| 1:3:5-01 | 1.8132-04 | 0.9996 | 0.0 | 5.5347-08 | 0.0 |
| WATER | 0.0 | 0.0 | 1.0000 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 2811.7695 | 1.5933+04 |
| METHANE | 0.0 | 0.0 | 0.0 | 1.1734+05 | 4.5631+04 |
| ETHANE | 0.0 | 0.0 | 0.0 | 2.0643+05 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 2.1899+04 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 8478.0651 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 2681.5743 | 0.0 |
| BENZENE | 7.1633+04 | 3.7936-07 | 0.0 | 9825.0998 | 0.0 |
| TOLUENE | 3.5346+04 | 1.7395-03 | 0.0 | 406.4449 | 0.0 |
| P-XYL-01 | 9324.6534 | 3.8973 | 0.0 | 3.7968 | 0.0 |
| 1:3:5-01 | 30.2652 | 1.1936+04 | 0.0 | 0.1114 | 0.0 |
| WATER | 0.0 | 0.0 | 1.9338+04 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 7.6019-03 | 0.2588 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.3172 | 0.7412 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.5581 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 5.9207-02 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 2.2921-02 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 7.2499-03 | 0.0 |
| BENZENE | 0.6158 | 3.1772-11 | 0.0 | 2.6563-02 | 0.0 |
| TOLUENE | 0.3038 | 1.4568-07 | 0.0 | 1.0989-03 | 0.0 |
| P-XYL-01 | 8.0154-02 | 3.2640-04 | 0.0 | 1.0265-05 | 0.0 |
| 1:3:5-01 | 2.6016-04 | 0.9997 | 0.0 | 3.0109-07 | 0.0 |
| WATER | 0.0 | 0.0 | 1.0000 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 1388.7340 | 99.3452 | 1073.4269 | 1.6741+04 | 1.0748+04 |
| LB/HR | 1.1633+05 | 1.1940+04 | 1.9338+04 | 3.6988+05 | 6.1564+04 |
| CUFT/HR | 2234.7351 | 230.2501 | 2327.6736 | 1.5084+05 | 3.7127+05 |
| STATE VARIABLES: | | | | | |
| TEMP F | 136.3993 | 144.3420 | 380.2914 | 181.1316 | 180.6861 |
| PRES PSIA | 25.0000 | 3.7500 | 196.0000 | 689.9998 | 200.0000 |
| VFRAC | 0.0 | 0.0 | 4.2023-02 | 1.0000 | 1.0000 |
| LFRAC | 1.0000 | 1.0000 | 0.9580 | 0.0 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | 1.6802+04 | -2.3793+04 | -1.1630+05 | -2.7248+04 | -7711.6697 |
| BTU/LB | 200.5672 | -197.9592 | -6455.7857 | -1233.2512 | -1346.3470 |
| BTU/HR | 2.3333+07 | -2.3637+06 | -1.2484+08 | -4.5615+08 | -8.2887+07 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -63.9918 | -127.9778 | -29.6377 | -31.0799 | -7.8360 |
| BTU/LB-R | -0.7639 | -1.0648 | -1.6451 | -1.4067 | -1.3680 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 0.6214 | 0.4315 | 0.4612 | 0.1110 | 2.8950-02 |
| LB/CUFT | 52.0574 | 51.8576 | 8.3079 | 2.4522 | 0.1658 |
| AVG MW | 83.7702 | 120.1891 | 18.0153 | 22.0943 | 5.7278 |

S-219, S-220 S-220, S-221 S-221,
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| STREAM ID | S-219, | S-220 | S-220, | S-221 | S-221, |
|---|---|---|---|---|---|
| FROM : | PR-201 | V-206 | V-103 | V-206 | V-404 |
| TO : | PR-201, | V-103 | F-101 | V-404 | F-401-2 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | VAPOR | VAPOR | VAPOR | VAPOR |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 7903.9232 | 1388.6102 | 1388.6102 | 6515.3130 | 6515.3130 |
| METHANE | 2844.3385 | 499.7110 | 499.7110 | 2344.6275 | 2344.6275 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 2032.4726 | 0.0 | 9536.2938 |
| NITROGEN | 0.0 | 0.0 | 7645.9682 | 0.0 | 3.5875+04 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.7354 | 0.7354 | 0.1201 | 0.7354 | 0.1201 |
| METHANE | 0.2646 | 0.2646 | 4.3202-02 | 0.2646 | 4.3202-02 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.1757 | 0.0 | 0.1757 |
| NITROGEN | 0.0 | 0.0 | 0.6610 | 0.0 | 0.6610 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 1.5933+04 | 2799.2715 | 2799.2715 | 1.3134+04 | 1.3134+04 |
| METHANE | 4.5631+04 | 8016.7439 | 8016.7439 | 3.7614+04 | 3.7614+04 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 6.5037+04 | 0.0 | 3.0515+05 |
| NITROGEN | 0.0 | 0.0 | 2.1419+05 | 0.0 | 1.0050+06 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.2588 | 0.2588 | 9.6512-03 | 0.2588 | 9.6512-03 |
| METHANE | 0.7412 | 0.7412 | 2.7640-02 | 0.7412 | 2.7640-02 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| OXYGEN | 0.0 | 0.0 | 0.2242 | 0.0 | 0.2242 |
| NITROGEN | 0.0 | 0.0 | 0.7385 | 0.0 | 0.7385 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 1.0748+04 | 1888.3212 | 1.1567+04 | 8859.9405 | 5.4271+04 |
| LB/HR | 6.1564+04 | 1.0816+04 | 2.9004+05 | 5.0748+04 | 1.3609+06 |
| CUFT/HR | 1.0918+05 | 6.5226+04 | 4.7441+06 | 3.0604+05 | 2.2259+07 |
| STATE VARIABLES: | | | | | |
| TEMP F | 181.1316 | 180.6861 | 94.7830 | 180.6861 | 94.7830 |
| PRES PSIA | 689.9998 | 200.0000 | 14.5038 | 200.0000 | 14.5038 |
| VFRAC | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| LFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -7711.6697 | -7711.6697 | -1261.3801 | -7711.6697 | -1261.3801 |
| BTU/LB | -1346.3470 | -1346.3470 | -50.3032 | -1346.3470 | -50.3032 |
| BTU/HR | -8.2887+07 | -1.4562+07 | -1.4590+07 | -6.8325+07 | -6.8456+07 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -10.3217 | -7.8360 | 1.3451 | -7.8360 | 1.3451 |
| BTU/LB-R | -1.8020 | -1.3680 | 5.3641-02 | -1.3680 | 5.3641-02 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 9.8443-02 | 2.8950-02 | 2.4381-03 | 2.8950-02 | 2.4381-03 |
| LB/CUFT | 0.5639 | 0.1658 | 6.1138-02 | 0.1658 | 6.1138-02 |
| AVG MW | 5.7278 | 5.7278 | 25.0755 | 5.7278 | 25.0755 |

S-305 S-308 S-309 S-314 S-317
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| STREAM ID | S-305 | S-308 | S-309 | S-314 | S-317 |
|---|---|---|---|---|---|
| FROM : | COL-301 | RB-301 | COL-301 | COL-302 | RB-302 |
| TO : | T-103 | V-401-3 | COL-302 | H-201 | V-401-3 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | MIXED | LIQUID | LIQUID | MIXED |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 5.2075-05 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 172.6175 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 238.5242 | 0.0 | 1.2669-29 | 0.0 | 0.0 |
| ETHENE | 22.0910 | 0.0 | 2.9603-33 | 0.0 | 0.0 |
| PROPANE | 16.4274 | 0.0 | 5.5478-23 | 0.0 | 0.0 |
| PROPENE | 3.4654 | 0.0 | 5.8969-30 | 0.0 | 0.0 |
| BENZENE | 108.5439 | 0.0 | 917.0410 | 917.0410 | 0.0 |
| TOLUENE | 10.4562 | 0.0 | 383.6115 | 383.6114 | 0.0 |
| P-XYL-01 | 0.1014 | 0.0 | 87.8664 | 87.8297 | 0.0 |
| 1:3:5-01 | 1.8392-07 | 0.0 | 99.5603 | 0.2518 | 0.0 |
| WATER | 0.0 | 646.0829 | 0.0 | 0.0 | 2074.3381 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| HYDROGEN | 9.1005-08 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.3017 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.4168 | 0.0 | 8.5135-33 | 0.0 | 0.0 |
| ETHENE | 3.8605-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 2.8708-02 | 0.0 | 3.7282-26 | 0.0 | 0.0 |
| PROPENE | 6.0559-03 | 0.0 | 3.9628-33 | 0.0 | 0.0 |
| BENZENE | 0.1897 | 0.0 | 0.6163 | 0.6603 | 0.0 |
| TOLUENE | 1.8273-02 | 0.0 | 0.2578 | 0.2762 | 0.0 |
| P-XYL-01 | 1.7728-04 | 0.0 | 5.9047-02 | 6.3244-02 | 0.0 |
| 1:3:5-01 | 3.2141-10 | 0.0 | 6.6905-02 | 1.8132-04 | 0.0 |
| WATER | 0.0 | 1.0000 | 0.0 | 0.0 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 1.0498-04 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 2769.2615 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 7172.3375 | 0.0 | 3.8095-28 | 0.0 | 0.0 |
| ETHENE | 619.7359 | 0.0 | 8.3046-32 | 0.0 | 0.0 |
| PROPANE | 724.3933 | 0.0 | 2.4464-21 | 0.0 | 0.0 |
| PROPENE | 145.8246 | 0.0 | 2.4815-28 | 0.0 | 0.0 |
| BENZENE | 8478.7610 | 0.0 | 7.1633+04 | 7.1633+04 | 0.0 |
| TOLUENE | 963.4368 | 0.0 | 3.5346+04 | 3.5346+04 | 0.0 |
| P-XYL-01 | 10.7700 | 0.0 | 9328.5507 | 9324.6534 | 0.0 |
| 1:3:5-01 | 2.2106-05 | 0.0 | 1.1967+04 | 30.2652 | 0.0 |
| WATER | 0.0 | 1.1639+04 | 0.0 | 0.0 | 3.7370+04 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 5.0266-09 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.1326 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.3434 | 0.0 | 2.9698-33 | 0.0 | 0.0 |
| ETHENE | 2.9674-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 3.4686-02 | 0.0 | 1.9071-26 | 0.0 | 0.0 |
| PROPENE | 6.9824-03 | 0.0 | 1.9345-33 | 0.0 | 0.0 |
| BENZENE | 0.4060 | 0.0 | 0.5584 | 0.6158 | 0.0 |
| TOLUENE | 4.6132-02 | 0.0 | 0.2756 | 0.3038 | 0.0 |
| P-XYL-01 | 5.1570-04 | 0.0 | 7.2723-02 | 8.0154-02 | 0.0 |
| 1:3:5-01 | 1.0585-09 | 0.0 | 9.3289-02 | 2.6016-04 | 0.0 |
| WATER | 0.0 | 1.0000 | 0.0 | 0.0 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 572.2272 | 646.0829 | 1488.0792 | 1388.7340 | 2074.3381 |
| LB/HR | 2.0885+04 | 1.1639+04 | 1.2827+05 | 1.1633+05 | 3.7370+04 |
| CUFT/HR | 4.6730+04 | 1400.9990 | 2583.3950 | 2431.5464 | 4498.1002 |
| STATE VARIABLES: | | | | | |
| TEMP F | 193.0605 | 380.2914 | 200.4235 | 249.7144 | 380.2914 |
| PRES PSIA | 83.0000 | 196.0000 | 16.0000 | 35.0000 | 196.0000 |
| VFRAC | 1.0000 | 4.2023-02 | 0.0 | 0.0 | 4.2023-02 |
| LFRAC | 0.0 | 0.9580 | 1.0000 | 1.0000 | 0.9580 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -1.6391+04 | -1.1630+05 | 1.6683+04 | 2.1466+04 | -1.1630+05 |
| BTU/LB | -449.1031 | -6455.7857 | 193.5382 | 256.2534 | -6455.7857 |

| | | | | | |
|---|---|---|---|---|---|
| BTU/HR | -9.3793+06 | -7.5141+07 | 2.4826+07 | 2.9811+07 | -2.4125+08 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -31.9389 | -29.6377 | -63.6657 | -56.8798 | -29.6377 |
| BTU/LB-R | -0.8751 | -1.6451 | -0.7386 | -0.6790 | -1.6451 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 1.2245-02 | 0.4612 | 0.5760 | 0.5711 | 0.4612 |
| LB/CUFT | 0.4469 | 8.3079 | 49.6535 | 47.8438 | 8.3079 |
| AVG MW | 36.4969 | 18.0153 | 86.2015 | 83.7702 | 18.0153 |

S-318 S-401 S-402 S-403 S-404
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| STREAM ID | S-318 | S-401 | S-402 | S-403 | S-404 |
|---|---|---|---|---|---|
| FROM : | COL-302 | ---- | P-401 | V-401-3 | F-401-2, |
| TO : | H-202 | P-401 | V-401-3 | F-401-2, | V-405 |
| MAX CONV. ERROR: | 0.0 | 0.0 | 0.0 | 0.0 | 1.3755-08 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | LIQUID | LIQUID | LIQUID | LIQUID | VAPOR |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 4.8566-09 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 1.8879-05 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 3.6709-02 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 99.3085 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 5.7897+04 | 5.7897+04 | 6.1691+04 | 6.1691+04 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 4.8886-11 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 1.9003-07 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 3.6951-04 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.9996 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| BENZENE | 3.7936-07 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 1.7395-03 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 3.8973 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 1.1936+04 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 1.0430+06 | 1.0430+06 | 1.1114+06 | 1.1114+06 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 3.1772-11 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 1.4568-07 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 3.2640-04 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.9997 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 0.0 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 99.3452 | 5.7897+04 | 5.7897+04 | 6.1691+04 | 6.1691+04 |
| LB/HR | 1.1940+04 | 1.0430+06 | 1.0430+06 | 1.1114+06 | 1.1114+06 |
| CUFT/HR | 259.3541 | 1.6809+04 | 1.6811+04 | 1.8136+04 | 1.1820+06 |
| STATE VARIABLES: | | | | | |
| TEMP F | 323.7883 | 77.0000 | 77.2090 | 99.9141 | 465.2781 |
| PRES PSIA | 13.7500 | 14.5038 | 205.6316 | 196.0000 | 464.6959 |
| VFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 1.0000 |
| LFRAC | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -1.3382+04 | -1.2287+05 | -1.2286+05 | -1.2246+05 | -1.0130+05 |
| BTU/LB | -111.3439 | -6820.4540 | -6819.7415 | -6797.3592 | -5623.1311 |
| BTU/HR | -1.3295+06 | -7.1140+09 | -7.1132+09 | -7.5545+09 | -6.2494+09 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -112.9853 | -38.9666 | -38.9618 | -38.2274 | -13.3860 |
| BTU/LB-R | -0.9401 | -2.1630 | -2.1627 | -2.1219 | -0.7430 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 0.3830 | 3.4443 | 3.4439 | 3.4015 | 5.2194-02 |
| LB/CUFT | 46.0383 | 62.0507 | 62.0437 | 61.2788 | 0.9403 |
| AVG MW | 120.1891 | 18.0153 | 18.0153 | 18.0153 | 18.0153 |

S-404, S-405 S-406 S-407 S-408
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| STREAM ID | S-404, | S-405 | S-406 | S-407 | S-408 |
|---|---|---|---|---|---|
| FROM : | V-405 | V-405 | T-401 | V-406-7 | V-406-7 |
| TO : | T-401 | ---- | V-406-7 | H-203, | RB-301 |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | VAPOR | VAPOR | MIXED | MIXED | MIXED |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 3793.8480 | 5.7897+04 | 3793.8480 | 1073.4269 | 646.0829 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 6.8347+04 | 1.0430+06 | 6.8347+04 | 1.9338+04 | 1.1639+04 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 3793.8480 | 5.7897+04 | 3793.8480 | 1073.4269 | 646.0829 |
| LB/HR | 6.8347+04 | 1.0430+06 | 6.8347+04 | 1.9338+04 | 1.1639+04 |
| CUFT/HR | 7.2687+04 | 1.1093+06 | 1.5112+05 | 4.2759+04 | 2.5736+04 |
| STATE VARIABLES: | | | | | |
| TEMP F | 465.2779 | 465.2779 | 384.4670 | 384.4670 | 384.4670 |
| PRES PSIA | 464.6959 | 464.6959 | 206.0000 | 206.0000 | 206.0000 |
| VFRAC | 1.0000 | 1.0000 | 0.9597 | 0.9597 | 0.9597 |
| LFRAC | 0.0 | 0.0 | 4.0290-02 | 4.0290-02 | 4.0290-02 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -1.0130+05 | -1.0130+05 | -1.0232+05 | -1.0232+05 | -1.0232+05 |
| BTU/LB | -5623.1311 | -5623.1311 | -5679.7743 | -5679.7743 | -5679.7743 |
| BTU/HR | -3.8433+08 | -5.8651+09 | -3.8820+08 | -1.0984+08 | -6.6109+07 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -13.3860 | -13.3860 | -13.0838 | -13.0838 | -13.0838 |
| BTU/LB-R | -0.7430 | -0.7430 | -0.7263 | -0.7263 | -0.7263 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 5.2194-02 | 5.2194-02 | 2.5104-02 | 2.5104-02 | 2.5104-02 |
| LB/CUFT | 0.9403 | 0.9403 | 0.4523 | 0.4523 | 0.4523 |
| AVG MW | 18.0153 | 18.0153 | 18.0153 | 18.0153 | 18.0153 |

S-409 S-410 S-411 S1 S2
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| STREAM ID | S-409 | S-410 | S-411 | S1 | S2 |
|---|---|---|---|---|---|
| FROM : | V-406-7 | ---- | F-401-2 | ---- | BOCKRATH |
| TO : | RB-302 | V-404 | ---- | BOCKRATH | ---- |
| SUBSTREAM: MIXED | | | | | |
| PHASE: | MIXED | VAPOR | VAPOR | LIQUID | VAPOR |
| COMPONENTS: LBMOL/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 2074.3381 | 0.0 | 1.1205+04 | 9158.8918 | 9158.8918 |
| OXYGEN | 0.0 | 9536.2938 | 1589.3823 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 3.5875+04 | 3.5875+04 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 2344.6275 | 0.0 | 0.0 |
| COMPONENTS: MOLE FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

| | | | | | |
|---|---|---|---|---|---|
| WATER | 1.0000 | 0.0 | 0.2196 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.2100 | 3.1156-02 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.7900 | 0.7032 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 4.5961-02 | 0.0 | 0.0 |
| COMPONENTS: LB/HR | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 3.7370+04 | 0.0 | 2.0185+05 | 1.6500+05 | 1.6500+05 |
| OXYGEN | 0.0 | 3.0515+05 | 5.0858+04 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 1.0050+06 | 1.0050+06 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 1.0319+05 | 0.0 | 0.0 |
| COMPONENTS: MASS FRAC | | | | | |
| HYDROGEN | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| METHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ETHENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPANE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| PROPENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BENZENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| TOLUENE | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| P-XYL-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1:3:5-01 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| WATER | 1.0000 | 0.0 | 0.1483 | 1.0000 | 1.0000 |
| OXYGEN | 0.0 | 0.2329 | 3.7372-02 | 0.0 | 0.0 |
| NITROGEN | 0.0 | 0.7671 | 0.7385 | 0.0 | 0.0 |
| CARBO-01 | 0.0 | 0.0 | 7.5824-02 | 0.0 | 0.0 |
| TOTAL FLOW: | | | | | |
| LBMOL/HR | 2074.3381 | 4.5411+04 | 5.1013+04 | 9158.8918 | 9158.8918 |
| LB/HR | 3.7370+04 | 1.3101+06 | 1.3609+06 | 1.6500+05 | 1.6500+05 |
| CUFT/HR | 8.2629+04 | 1.8024+07 | 3.8936+07 | 2659.1155 | 6.5896+05 |
| STATE VARIABLES: | | | | | |
| TEMP F | 384.4670 | 77.0000 | 572.0000 | 77.0000 | 338.0404 |
| PRES PSIA | 206.0000 | 14.5038 | 14.5038 | 14.5000 | 114.6959 |
| VFRAC | 0.9597 | 1.0000 | 1.0000 | 0.0 | 1.0000 |
| LFRAC | 4.0290-02 | 0.0 | 0.0 | 1.0000 | 0.0 |
| SFRAC | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| ENTHALPY: | | | | | |
| BTU/LBMOL | -1.0232+05 | -2.8903 | -2.6924+04 | -1.2287+05 | -1.0199+05 |
| BTU/LB | -5679.7743 | -0.1002 | -1009.2589 | -6820.4540 | -5661.5602 |
| BTU/HR | -2.1225+08 | -1.3125+05 | -1.3735+09 | -1.1254+09 | -9.3416+08 |
| ENTROPY: | | | | | |
| BTU/LBMOL-R | -13.0838 | 1.0423 | 4.2301 | -38.9666 | -11.5948 |
| BTU/LB-R | -0.7263 | 3.6128-02 | 0.1586 | -2.1630 | -0.6436 |
| DENSITY: | | | | | |
| LBMOL/CUFT | 2.5104-02 | 2.5195-03 | 1.3102-03 | 3.4443 | 1.3899-02 |
| LB/CUFT | 0.4523 | 7.2689-02 | 3.4951-02 | 62.0507 | 0.2504 |
| AVG MW | 18.0153 | 28.8504 | 26.6768 | 18.0153 | 18.0153 |

### *A-5.3. Block Report*

```
BLOCK:  C-201-3  MODEL: MCOMPR
------------------------------
  INLET STREAMS:     S-108        TO STAGE   1
  OUTLET STREAMS:    S-201      FROM STAGE   4
                     S-204      FROM STAGE   1
                     S-203      FROM STAGE   2
                     S-202      FROM STAGE   3
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                      ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            29549.4         29549.4         0.00000
      MASS(LB/HR   )            580601.         580601.       -0.200508E-15
      ENTHALPY(BTU/HR  )      -0.524333E+09   -0.553627E+09    0.529134E-01

                      ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.414343E+07  LB/HR
   PRODUCT STREAMS CO2E         0.414343E+07  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 CENTRIFUGAL COMPRESSOR
  NUMBER OF STAGES                                                4

                    COMPRESSOR SPECIFICATIONS PER STAGE

  STAGE     PRESSURE        MECHANICAL      ISENTROPIC
  NUMBER    RATIO           EFFICIENCY      EFFICIENCY

    1       2.465             1.000         0.8000
    2       2.465             1.000         0.8000
    3       2.465             1.000         0.8000
    4       2.465             1.000         0.8000

                    COOLER SPECIFICATIONS PER STAGE

  STAGE     PRESSURE DROP     TEMPERATURE
  NUMBER    PSI               F

    1       10.00             104.0
    2       10.00             104.0
    3       10.00             104.0
    4       10.00             104.0

                           ***  RESULTS  ***

  FINAL PRESSURE, PSIA                                          730.000
  TOTAL WORK REQUIRED, HP                                    61,139.0
  TOTAL COOLING DUTY , BTU/HR                                    -0.184859+09
```

*** PROFILE ***

COMPRESSOR PROFILE

| STAGE NUMBER | OUTLET PRESSURE PSIA | PRESSURE RATIO | OUTLET TEMPERATURE F |
|---|---|---|---|
| 1 | 65.11 | 2.465 | 218.2 |
| 2 | 135.8 | 2.465 | 238.1 |
| 3 | 310.2 | 2.465 | 242.2 |
| 4 | 740.0 | 2.465 | 246.2 |

| STAGE NUMBER | INDICATED HORSEPOWER HP | BRAKE HORSEPOWER HP |
|---|---|---|
| 1 | 0.1557E+05 | 0.1557E+05 |
| 2 | 0.1555E+05 | 0.1555E+05 |
| 3 | 0.1521E+05 | 0.1521E+05 |
| 4 | 0.1481E+05 | 0.1481E+05 |

| STAGE NUMBER | HEAD DEVELOPED FT-LBF/LB | VOLUMETRIC FLOW CUFT/HR | ISENTROPIC EFFICIENCY |
|---|---|---|---|
| 1 | 0.4248E+05 | 0.6585E+07 | 0.8000 |
| 2 | 0.4756E+05 | 0.3143E+07 | 0.8000 |
| 3 | 0.5031E+05 | 0.1343E+07 | 0.8000 |
| 4 | 0.5221E+05 | 0.5456E+06 | 0.8000 |

COOLER PROFILE

| STAGE NUMBER | OUTLET TEMPERATURE F | OUTLET PRESSURE PSIA | COOLING LOAD BTU/HR | VAPOR FRACTION |
|---|---|---|---|---|
| 1 | 104.0 | 55.11 | -.4709E+08 | 0.9755 |
| 2 | 104.0 | 125.8 | -.4720E+08 | 0.9822 |
| 3 | 104.0 | 300.2 | -.4564E+08 | 0.9838 |
| 4 | 104.0 | 730.0 | -.4492E+08 | 0.9869 |

BLOCK: COL-201 MODEL: FLASH2

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

INLET STREAM: S-201
OUTLET VAPOR STREAM: S-211
OUTLET LIQUID STREAM: S-205
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***

| | IN | OUT | RELATIVE DIFF. |
|---|---|---|---|
| TOTAL BALANCE | | | |
| MOLE(LBMOL/HR) | 27854.9 | 27854.9 | -0.576129E-06 |
| MASS(LB/HR ) | 449349. | 449349. | -0.485841E-06 |
| ENTHALPY(BTU/HR ) | -0.563270E+09 | -0.563271E+09 | 0.825102E-06 |

*** CO2 EQUIVALENT SUMMARY ***

| | | |
|---|---|---|
| FEED STREAMS CO2E | 0.410732E+07 | LB/HR |
| PRODUCT STREAMS CO2E | 0.410733E+07 | LB/HR |

```
 NET STREAMS CO2E PRODUCTION   6.94591      LB/HR
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION         6.94591      LB/HR

                       ***  INPUT DATA  ***
TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                   104.000
PRESSURE DROP         PSI                                   0.0
MAXIMUM NO. ITERATIONS                                    30
CONVERGENCE TOLERANCE                                       0.000100000

                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                     104.00
OUTLET PRESSURE       PSIA                                  730.00
HEAT DUTY             BTU/HR                                0.60578E-01
VAPOR FRACTION                                              0.98687


V-L PHASE EQUILIBRIUM :

   COMP              F(I)          X(I)          Y(I)          K(I)
   HYDROGEN                0.33383             0.74795E-07       0.33827
0.45226E+07
   METHANE          0.36765       0.22583       0.36954        1.6363
   ETHANE           0.25017       0.28241       0.24974       0.88434
   ETHENE           0.28376E-01   0.26799E-01   0.28397E-01    1.0596
   PROPANE          0.71497E-02   0.18840E-01   0.69941E-02   0.37124
   PROPENE          0.23436E-02   0.42511E-02   0.23182E-02   0.54531
   BENZENE           0.98057E-02   0.40285        0.45756E-02    0.11358E-
01
   TOLUENE           0.65918E-03   0.38137E-01    0.16047E-03    0.42077E-
02
   P-XYL-01          0.12166E-04   0.82867E-03    0.13010E-05    0.15700E-
02
   1:3:5-01          0.77842E-06   0.56744E-04    0.33707E-07    0.59402E-
03

BLOCK:  COL-301  MODEL: RADFRAC
-------------------------------
   INLETS   - S-210    STAGE  14
   OUTLETS  - S-305    STAGE   1
              S-309    STAGE  42
              HEAT3    STAGE  42
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           2060.31         2060.31         0.00000
      MASS(LB/HR   )           149159.         149159.       -0.235430E-07
      ENTHALPY(BTU/HR  )     0.597939E+07    0.641447E+07   -0.678283E-01

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             69231.5      LB/HR
   PRODUCT STREAMS CO2E          69231.5      LB/HR
   NET STREAMS CO2E PRODUCTION -0.854772E-02  LB/HR
```

```
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION       -0.854772E-02  LB/HR



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

****   INPUT PARAMETERS   ****

 NUMBER OF STAGES                                               42
 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
 MASS REFLUX RATIO                                               0.10288
 MASS DISTILLATE TO FEED RATIO                                   0.14001

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIA                          83.0000
                         2                                      10.0000

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


***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
              S-305        S-309
 COMPONENT:
 HYDROGEN    1.0000       0.0000
 METHANE     1.0000       0.0000
 ETHANE      1.0000       0.0000
 ETHENE      1.0000       0.0000
 PROPANE     1.0000       0.0000
 PROPENE     1.0000       0.0000
 BENZENE     .10584       .89416
 TOLUENE     .26534E-01   .97347
 P-XYL-01    .11532E-02   .99885
 1:3:5-01    .18473E-08   1.0000
```

*** SUMMARY OF KEY RESULTS ***

| | | |
|---|---|---|
| TOP STAGE TEMPERATURE | F | 193.060 |
| BOTTOM STAGE TEMPERATURE | F | 200.424 |
| TOP STAGE LIQUID FLOW | LBMOL/HR | 28.0315 |
| BOTTOM STAGE LIQUID FLOW | LBMOL/HR | 1,488.08 |
| TOP STAGE VAPOR FLOW | LBMOL/HR | 572.227 |
| BOILUP VAPOR FLOW | LBMOL/HR | 653.807 |
| MOLAR REFLUX RATIO | | 0.048987 |
| MOLAR BOILUP RATIO | | 0.43936 |
| CONDENSER DUTY (W/O SUBCOOL) | BTU/HR | 435,077. |
| REBOILER DUTY | BTU/HR | 9,032,280. |

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

| | | |
|---|---|---|
| DEW POINT | 0.21263E-05 | STAGE= 1 |
| BUBBLE POINT | 0.59084E-05 | STAGE= 3 |
| COMPONENT MASS BALANCE | 0.16503E-05 | STAGE= 16 COMP=METHANE |
| ENERGY BALANCE | 0.25582E-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 | 193.06 | 83.000 | 17570. | -16391. | .43508+06 |
| 2 | 96.784 | 10.000 | 16166. | -15530. | |
| 12 | 102.99 | 11.500 | 14577. | -16255. | |
| 13 | 103.91 | 11.650 | 14053. | -16287. | |
| 14 | 157.25 | 11.800 | 16054. | 14238. | |
| 15 | 176.73 | 11.950 | 17480. | 33700. | |
| 39 | 193.92 | 15.550 | 18427. | 36227. | |
| 40 | 194.59 | 15.700 | 18429. | 36226. | |
| 41 | 195.72 | 15.850 | 18275. | 36163. | |
| 42 | 200.42 | 16.000 | 16683. | 35714. | .90323+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 | | 28.03 | | | | | 572.2 572.2271 |
| 2 | 19.69 | 600.3 | | | | | |
| 12 | 16.01 | 588.7 | | | | | |
| 13 | 17.78 | 588.2 | | 462.8550 | | | |
| 14 | 1947. | 127.2 | 1597.4512 | | | | |
| 15 | 2049. | 458.8 | | | | | |
| 39 | 2141. | 650.1 | | | | | |
| 40 | 2144. | 653.2 | | | | | |
| 41 | 2142. | 655.8 | | | | | |
| 42 | 1488. | 653.8 | | | | 1488.0792 | |

**** 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 | | 2149. | | | | | 0.2088E+05 .20885+05 |
| 2 | 1600. | 0.2303E+05 | | | | | |
| 12 | 1324. | 0.2225E+05 | | | | | |
| 13 | 1478. | 0.2221E+05 | | .14236+05 | | | |
| 14 | 0.1643E+06 | 8127. | .13492+06 | | | | |
| 15 | 0.1731E+06 | 0.3606E+05 | | | | | |
| 39 | 0.1806E+06 | 0.5208E+05 | | | | | |
| 40 | 0.1809E+06 | 0.5233E+05 | | | | | |
| 41 | 0.1811E+06 | 0.5260E+05 | | | | | |
| 42 | 0.1283E+06 | 0.5283E+05 | | | | .12827+06 | |

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

| STAGE | HYDROGEN | METHANE | ETHANE | ETHENE | PROPANE |
|---|---|---|---|---|---|
| 1 | 0.88549E-14 | 0.11043E-01 | 0.58174E-01 | 0.44557E-02 | 0.70493E-02 |
| 2 | 0.24465E-15 | 0.32870E-02 | 0.10857E-01 | 0.80200E-03 | 0.19598E-02 |
| 12 | 0.31759E-15 | 0.37860E-02 | 0.12317E-01 | 0.90227E-03 | 0.21132E-02 |
| 13 | 0.32645E-15 | 0.38248E-02 | 0.12417E-01 | 0.90883E-03 | 0.21170E-02 |
| 14 | 0.27575E-22 | 0.48442E-03 | 0.47760E-02 | 0.30069E-03 | 0.16300E-02 |
| 15 | 0.13229E-29 | 0.13120E-04 | 0.45753E-03 | 0.23410E-04 | 0.28654E-03 |
| 39 | 0.14121-204 | 0.54073E-44 | 0.12277E-28 | 0.50725E-32 | 0.10119E-22 |
| 40 | 0.86934-212 | 0.12405E-45 | 0.11112E-29 | 0.37763E-33 | 0.16260E-23 |
| 41 | 0.54660-219 | 0.28322E-47 | 0.10034E-30 | 0.28110E-34 | 0.25825E-24 |
| 42 | 0.36824-226 | 0.61458E-49 | 0.85135E-32 | 0.19893E-35 | 0.37282E-25 |

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

| STAGE | PROPENE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|---|
| 1 | 0.89414E-03 | 0.74353 | 0.17072 | 0.41364E-02 | 0.17122E-07 |
| 2 | 0.22921E-03 | 0.71023 | 0.26044 | 0.12196E-01 | 0.11530E-06 |
| 12 | 0.25717E-03 | 0.66520 | 0.24836 | 0.57667E-01 | 0.93962E-02 |
| 13 | 0.25863E-03 | 0.65819 | 0.24296 | 0.54913E-01 | 0.24408E-01 |
| 14 | 0.13475E-03 | 0.67133 | 0.22218 | 0.47124E-01 | 0.52040E-01 |
| 15 | 0.14337E-04 | 0.68700 | 0.21726 | 0.45271E-01 | 0.49676E-01 |
| 39 | 0.39239E-29 | 0.69517 | 0.21322 | 0.43806E-01 | 0.47801E-01 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 0.39454E-30 | 0.69351 | 0.21482 | 0.43881E-01 | 0.47790E-01 |
| 41 | 0.39919E-31 | 0.68295 | 0.22339 | 0.45130E-01 | 0.48526E-01 |
| 42 | 0.39628E-32 | 0.61626 | 0.25779 | 0.59047E-01 | 0.66905E-01 |

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

| STAGE | HYDROGEN | METHANE | ETHANE | ETHENE | PROPANE |
|---|---|---|---|---|---|
| 1 | 0.91005E-07 | 0.30166 | 0.41683 | 0.38605E-01 | 0.28708E-01 |
| 2 | 0.86755E-07 | 0.28809 | 0.40009 | 0.37011E-01 | 0.27696E-01 |
| 12 | 0.88452E-07 | 0.29330 | 0.40548 | 0.37548E-01 | 0.27962E-01 |
| 13 | 0.88527E-07 | 0.29355 | 0.40582 | 0.37579E-01 | 0.27984E-01 |
| 14 | 0.32385E-14 | 0.62693E-01 | 0.19776 | 0.15503E-01 | 0.34794E-01 |
| 15 | 0.11701E-21 | 0.20556E-02 | 0.20266E-01 | 0.12759E-02 | 0.69167E-02 |
| 39 | 0.76572-197 | 0.77489E-42 | 0.44758E-27 | 0.22496E-30 | 0.20723E-21 |
| 40 | 0.46289-204 | 0.17725E-43 | 0.40226E-28 | 0.16623E-31 | 0.33085E-22 |
| 41 | 0.28420-211 | 0.40539E-45 | 0.36133E-29 | 0.12300E-32 | 0.52310E-23 |
| 42 | 0.17907-218 | 0.91386E-47 | 0.30932E-30 | 0.87560E-34 | 0.76119E-24 |

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

| STAGE | PROPENE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|---|
| 1 | 0.60559E-02 | 0.18969 | 0.18273E-01 | 0.17728E-03 | 0.32141E-09 |
| 2 | 0.58149E-02 | 0.21555 | 0.25392E-01 | 0.36217E-03 | 0.11060E-08 |
| 12 | 0.58932E-02 | 0.20310 | 0.24813E-01 | 0.18042E-02 | 0.96641E-04 |
| 13 | 0.58980E-02 | 0.20263 | 0.24537E-01 | 0.17424E-02 | 0.25581E-03 |
| 14 | 0.47962E-02 | 0.60069 | 0.75464E-01 | 0.57916E-02 | 0.25025E-02 |
| 15 | 0.57180E-03 | 0.84995 | 0.10668 | 0.84543E-02 | 0.38282E-02 |
| 39 | 0.12916E-27 | 0.87611 | 0.11060 | 0.90366E-02 | 0.42565E-02 |
| 40 | 0.12853E-28 | 0.87494 | 0.11169 | 0.90883E-02 | 0.42804E-02 |
| 41 | 0.12808E-29 | 0.86880 | 0.11732 | 0.94668E-02 | 0.44165E-02 |
| 42 | 0.12176E-30 | 0.83475 | 0.14510 | 0.13455E-01 | 0.66935E-02 |

**** K-VALUES ****

| STAGE | HYDROGEN | METHANE | ETHANE | ETHENE | PROPANE |
|---|---|---|---|---|---|
| 1 | 0.10277E+08 | 27.316 | 7.1652 | 8.6641 | 4.0724 |
| 2 | 0.35461E+09 | 87.643 | 36.852 | 46.148 | 14.132 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 0.27851E+09 | 77.470 | 32.921 | 41.614 | 13.232 |
| 13 | 0.27118E+09 | 76.748 | 32.683 | 41.348 | 13.219 |
| 14 | 0.11744E+09 | 129.42 | 41.407 | 51.557 | 21.346 |
| 15 | 0.88450E+08 | 156.68 | 44.296 | 54.504 | 24.138 |
| 39 | 0.54224E+08 | 143.30 | 36.455 | 44.349 | 20.479 |
| 40 | 0.53247E+08 | 142.88 | 36.200 | 44.019 | 20.347 |
| 41 | 0.51993E+08 | 143.14 | 36.012 | 43.758 | 20.255 |
| 42 | 0.48628E+08 | 148.70 | 36.333 | 44.015 | 20.417 |

**** K-VALUES ****

| STAGE | PROPENE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|---|
| 1 | 6.7728 | 0.25512 | 0.10703 | 0.42859E-01 | 0.18773E-01 |
| 2 | 25.369 | 0.30349 | 0.97498E-01 | 0.29696E-01 | 0.95922E-02 |
| 12 | 22.916 | 0.30532 | 0.99907E-01 | 0.31287E-01 | 0.10285E-01 |
| 13 | 22.805 | 0.30786 | 0.10099 | 0.31731E-01 | 0.10481E-01 |
| 14 | 35.594 | 0.89478 | 0.33965 | 0.12290 | 0.48088E-01 |
| 15 | 39.882 | 1.2372 | 0.49103 | 0.18675 | 0.77064E-01 |
| 39 | 32.917 | 1.2603 | 0.51870 | 0.20629 | 0.89046E-01 |
| 40 | 32.578 | 1.2616 | 0.51991 | 0.20711 | 0.89566E-01 |
| 41 | 32.086 | 1.2721 | 0.52517 | 0.20977 | 0.91013E-01 |
| 42 | 30.725 | 1.3546 | 0.56285 | 0.22786 | 0.10005 |

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

| STAGE | HYDROGEN | METHANE | ETHANE | ETHENE | PROPANE |
|---|---|---|---|---|---|
| 1 | 0.23289E-15 | 0.23114E-02 | 0.22822E-01 | 0.16308E-02 | 0.40555E-02 |
| 2 | 0.60685E-17 | 0.64887E-03 | 0.40170E-02 | 0.27685E-03 | 0.10634E-02 |
| 12 | 0.77455E-17 | 0.73481E-03 | 0.44807E-02 | 0.30623E-03 | 0.11274E-02 |
| 13 | 0.79165E-17 | 0.73814E-03 | 0.44915E-02 | 0.30671E-03 | 0.11230E-02 |
| 14 | 0.65858E-24 | 0.92071E-04 | 0.17014E-02 | 0.99938E-04 | 0.85155E-03 |
| 15 | 0.31565E-31 | 0.24912E-05 | 0.16284E-03 | 0.77733E-05 | 0.14956E-03 |
| 39 | 0.33751-206 | 0.10285E-44 | 0.43770E-29 | 0.16872E-32 | 0.52903E-23 |
| 40 | 0.20772-213 | 0.23588E-46 | 0.39604E-30 | 0.12557E-33 | 0.84985E-24 |
| 41 | 0.13032-220 | 0.53736E-48 | 0.35681E-31 | 0.93262E-35 | 0.13468E-24 |
| 42 | 0.86116-228 | 0.11438E-49 | 0.29698E-32 | 0.64741E-36 | 0.19071E-25 |

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

| STAGE | PROPENE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 0.49089E-03 | 0.75774 | 0.20522 | 0.57294E-02 | 0.26849E-07 |
| 2 | 0.11868E-03 | 0.68266 | 0.29528 | 0.15932E-01 | 0.17053E-06 |
| 12 | 0.13092E-03 | 0.62863 | 0.27686 | 0.74068E-01 | 0.13663E-01 |
| 13 | 0.13092E-03 | 0.61849 | 0.26930 | 0.70132E-01 | 0.35291E-01 |
| 14 | 0.67179E-04 | 0.62127 | 0.24254 | 0.59273E-01 | 0.74105E-01 |
| 15 | 0.71409E-05 | 0.63517 | 0.23694 | 0.56888E-01 | 0.70670E-01 |
| 39 | 0.19577E-29 | 0.64382 | 0.23293 | 0.55140E-01 | 0.68117E-01 |
| 40 | 0.19679E-30 | 0.64209 | 0.23461 | 0.55218E-01 | 0.68083E-01 |
| 41 | 0.19866E-31 | 0.63093 | 0.24343 | 0.56665E-01 | 0.68979E-01 |
| 42 | 0.19345E-32 | 0.55844 | 0.27555 | 0.72723E-01 | 0.93289E-01 |

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

| STAGE | HYDROGEN | METHANE | ETHANE | ETHENE | PROPANE |
|---|---|---|---|---|---|
| 1 | 0.50266E-08 | 0.13260 | 0.34343 | 0.29674E-01 | 0.34686E-01 |
| 2 | 0.45577E-08 | 0.12045 | 0.31352 | 0.27058E-01 | 0.31828E-01 |
| 12 | 0.47189E-08 | 0.12453 | 0.32268 | 0.27876E-01 | 0.32631E-01 |
| 13 | 0.47270E-08 | 0.12474 | 0.32322 | 0.27924E-01 | 0.32685E-01 |
| 14 | 0.10214E-15 | 0.15736E-01 | 0.93039E-01 | 0.68045E-02 | 0.24005E-01 |
| 15 | 0.30016E-23 | 0.41963E-03 | 0.77545E-02 | 0.45548E-03 | 0.38811E-02 |
| 39 | 0.19271-198 | 0.15520E-42 | 0.16803E-27 | 0.78792E-31 | 0.11409E-21 |
| 40 | 0.11647-205 | 0.35493E-44 | 0.15098E-28 | 0.58208E-32 | 0.18210E-22 |
| 41 | 0.71425-213 | 0.81082E-46 | 0.13546E-29 | 0.43020E-33 | 0.28758E-23 |
| 42 | 0.44671-220 | 0.18143E-47 | 0.11510E-30 | 0.30398E-34 | 0.41538E-24 |

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

| STAGE | PROPENE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|---|
| 1 | 0.69824E-02 | 0.40598 | 0.46132E-01 | 0.51570E-03 | 0.10585E-08 |
| 2 | 0.63769E-02 | 0.43880 | 0.60972E-01 | 0.10020E-02 | 0.34643E-08 |
| 12 | 0.65629E-02 | 0.41985 | 0.60506E-01 | 0.50692E-02 | 0.30740E-03 |
| 13 | 0.65740E-02 | 0.41925 | 0.59884E-01 | 0.48999E-02 | 0.81442E-03 |
| 14 | 0.31578E-02 | 0.73414 | 0.10879 | 0.96203E-02 | 0.47061E-02 |

```
    15    0.30618E-03   0.84483       0.12508       0.11421E-01   0.58550E-
02
    39    0.67857E-28   0.85441       0.12722       0.11978E-01   0.63872E-
02
    40    0.67512E-29   0.85308       0.12845       0.12044E-01   0.64217E-
02
    41    0.67195E-30   0.84609       0.13477       0.12530E-01   0.66180E-
02
    42    0.63404E-31   0.80692       0.16545       0.17677E-01   0.99560E-
02

 BLOCK:  COL-302  MODEL: RADFRAC
 -------------------------------
    INLETS   - S-309    STAGE  15
    OUTLETS  - S-314    STAGE   1
               S-318    STAGE  27
               HEAT4    STAGE  27
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           1488.08         1488.08       -0.152797E-15
       MASS(LB/HR   )           128275.         128275.       -0.159352E-09
       ENTHALPY(BTU/HR  )       0.248261E+08    -517737.        1.02085

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

   ****   INPUT PARAMETERS   ****

    NUMBER OF STAGES                                      27
    ALGORITHM OPTION                                    STANDARD
    ABSORBER OPTION                                     NO
    INITIALIZATION OPTION                               STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                    NO
    INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
    DESIGN SPECIFICATION METHOD                         NESTED
    MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
    MAXIMUM NO. OF INSIDE LOOP ITERATIONS                 10
    MAXIMUM NUMBER OF FLASH ITERATIONS                    30
    FLASH TOLERANCE                                        0.000100000
    OUTSIDE LOOP CONVERGENCE TOLERANCE                     0.000100000

   ****   COL-SPECS   ****

    MOLAR VAPOR DIST / TOTAL DIST                          0.0
```

```
 MASS REFLUX RATIO                                                 0.64165
 MASS DISTILLATE TO FEED RATIO                                     0.90692

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIA                            35.0000
                         2                                        10.0000

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


***   COMPONENT SPLIT FRACTIONS   ***

                         OUTLET STREAMS
                         --------------
             S-314        S-318
 COMPONENT:
 BENZENE     1.0000       .52959E-11
 TOLUENE     1.0000       .49213E-07
 P-XYL-01    .99958       .41778E-03
 1:3:5-01    .25291E-02   .99747


***    SUMMARY OF KEY RESULTS    ***

 TOP STAGE TEMPERATURE          F                                249.714
 BOTTOM STAGE TEMPERATURE       F                                323.788
 TOP STAGE LIQUID FLOW          LBMOL/HR                         891.088
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                          99.3452
 TOP STAGE VAPOR FLOW           LBMOL/HR                           0.0
 BOILUP VAPOR FLOW              LBMOL/HR                       1,709.75
 MOLAR REFLUX RATIO                                                0.64165
 MOLAR BOILUP RATIO                                               17.2102
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                            -0.253438+08
 REBOILER DUTY                  BTU/HR                             0.289994+08

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

 DEW POINT                       0.12342E-04  STAGE= 12
 BUBBLE POINT                    0.79140E-05  STAGE= 12
 COMPONENT MASS BALANCE          0.20754E-06  STAGE=  6 COMP=1:3:5-01
 ENERGY BALANCE                  0.93082E-05  STAGE= 15


****    PROFILES   ****

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

                                       ENTHALPY
STAGE TEMPERATURE   PRESSURE           BTU/LBMOL          HEAT DUTY
     F              PSIA          LIQUID       VAPOR        BTU/HR

  1   249.71         35.000       21466.       36973.      -.25344+08
  2   187.19         10.000       12043.       32583.
```

| | | | | | |
|---|---|---|---|---|---|
| 3 | 197.61 | 10.150 | 9384.1 | 30990. | |
| 13 | 227.44 | 11.650 | 319.31 | 29091. | |
| 14 | 230.05 | 11.800 | -420.05 | 28954. | |
| 15 | 233.51 | 11.950 | -1188.0 | 28557. | |
| 16 | 277.59 | 12.100 | -8901.8 | 17347. | |
| 25 | 322.22 | 13.450 | -13469. | 3477.7 | |
| 26 | 323.02 | 13.600 | -13427. | 3502.1 | |
| 27 | 323.79 | 13.750 | -13382. | 3531.6 | .28999+08 |

| STAGE | FLOW RATE LBMOL/HR | | FEED RATE LBMOL/HR | | | PRODUCT RATE LBMOL/HR | |
|---|---|---|---|---|---|---|---|
| | LIQUID | VAPOR | LIQUID | VAPOR | MIXED | LIQUID | VAPOR |
| 1 | 2280. | 0.000 | | | | 1388.7339 | |
| 2 | 639.6 | 2280. | | | | | |
| 3 | 622.9 | 2028. | | | | | |
| 13 | 521.9 | 1920. | | | | | |
| 14 | 516.3 | 1911. | | 79.3889 | | | |
| 15 | 1729. | 1826. | 1408.6902 | | | | |
| 16 | 1733. | 1630. | | | | | |
| 25 | 1808. | 1707. | | | | | |
| 26 | 1809. | 1708. | | | | | |
| 27 | 99.35 | 1710. | | | | 99.3452 | |

**** MASS FLOW PROFILES ****

| STAGE | FLOW RATE LB/HR | | FEED RATE LB/HR | | | PRODUCT RATE LB/HR | |
|---|---|---|---|---|---|---|---|
| | LIQUID | VAPOR | LIQUID | VAPOR | MIXED | LIQUID | VAPOR |
| 1 | 0.1910E+06 | 0.000 | | | | .11633+06 | |
| 2 | 0.5759E+05 | 0.1910E+06 | | | | | |
| 3 | 0.5787E+05 | 0.1739E+06 | | | | | |
| 13 | 0.5343E+05 | 0.1702E+06 | | | | | |
| 14 | 0.5326E+05 | 0.1698E+06 | | 6414.8241 | | | |
| 15 | 0.1799E+06 | 0.1632E+06 | .12186+06 | | | | |
| 16 | 0.1964E+06 | 0.1679E+06 | | | | | |
| 25 | 0.2172E+06 | 0.2051E+06 | | | | | |
| 26 | 0.2174E+06 | 0.2053E+06 | | | | | |
| 27 | 0.1194E+05 | 0.2055E+06 | | | | .11940+05 | |

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

| STAGE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|
| 1 | 0.66034 | 0.27623 | 0.63244E-01 | 0.18132E-03 |
| 2 | 0.37831 | 0.39510 | 0.22505 | 0.15456E-02 |
| 3 | 0.28423 | 0.38064 | 0.33096 | 0.41750E-02 |
| 13 | 0.19921 | 0.22658 | 0.21974 | 0.35447 |
| 14 | 0.19461 | 0.21768 | 0.19540 | 0.39230 |
| 15 | 0.18345 | 0.21111 | 0.18076 | 0.42468 |
| 16 | 0.40730E-01 | 0.97437E-01 | 0.16816 | 0.69368 |
| 25 | 0.21096E-08 | 0.21952E-05 | 0.12300E-02 | 0.99877 |
| 26 | 0.32174E-09 | 0.64889E-06 | 0.67845E-03 | 0.99932 |
| 27 | 0.48886E-10 | 0.19003E-06 | 0.36951E-03 | 0.99963 |

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

| STAGE | BENZENE | TOLUENE | P-XYL-01 | 1:3:5-01 |
|---|---|---|---|---|
| 1 | 0.82629 | 0.15722 | 0.16461E-01 | 0.23347E-04 |
| 2 | 0.66034 | 0.27623 | 0.63244E-01 | 0.18132E-03 |
| 3 | 0.57141 | 0.31371 | 0.11427 | 0.61152E-03 |

```
   13    0.53444        0.26577        0.11544        0.84346E-01
   14    0.53438        0.26267        0.10599        0.96960E-01
   15    0.52106        0.26533        0.10280        0.11081
   16    0.19463        0.22397        0.19175        0.38964
   25    0.14666E-07    0.78369E-05    0.23227E-02    0.99767
   26    0.22294E-08    0.23118E-05    0.12800E-02    0.99872
   27    0.33759E-09    0.67555E-06    0.69641E-03    0.99930

                        ****   K-VALUES            ****
 STAGE     BENZENE       TOLUENE        P-XYL-01       1:3:5-01
    1      1.2513       0.56917        0.26027        0.12876
    2      1.7455       0.69915        0.28103        0.11732
    3      2.0104       0.82418        0.34526        0.14647
   13      2.6829        1.1730        0.52535        0.23794
   14      2.7459        1.2067        0.54243        0.24715
   15      2.8403        1.2568        0.56869        0.26093
   16      4.7788        2.2987         1.1403        0.56169
   25      6.9522        3.5700         1.8884        0.99890
   26      6.9294        3.5628         1.8867        0.99940
   27      6.9057        3.5550         1.8847        0.99967

                        ****   MASS-X-PROFILE      ****
 STAGE     BENZENE       TOLUENE        P-XYL-01       1:3:5-01
    1    0.61575        0.30383        0.80154E-01    0.26016E-03
    2    0.32822        0.40434        0.26537        0.20633E-02
    3    0.23896        0.37747        0.37817        0.54008E-02
   13    0.15200        0.20393        0.22789        0.41618
   14    0.14736        0.19443        0.20111        0.45709
   15    0.13777        0.18700        0.18450        0.49073
   16    0.28059E-01    0.79179E-01    0.15745        0.73531
   25    0.13712E-08    0.16831E-05    0.10866E-02    0.99891
   26    0.20911E-09    0.49748E-06    0.59933E-03    0.99940
   27    0.31772E-10    0.14568E-06    0.32640E-03    0.99967

                        ****   MASS-Y-PROFILE      ****
 STAGE     BENZENE       TOLUENE        P-XYL-01       1:3:5-01
    1    0.79900        0.17933        0.21634E-01    0.34738E-04
    2    0.61575        0.30383        0.80154E-01    0.26016E-03
    3    0.52055        0.33711        0.14148        0.85720E-03
   13    0.47103        0.27630        0.13829        0.11438
   14    0.46980        0.27239        0.12665        0.13116
   15    0.45537        0.27351        0.12210        0.14901
   16    0.14756        0.20030        0.19759        0.45454
   25    0.95341E-08    0.60094E-05    0.20522E-02    0.99794
   26    0.14491E-08    0.17725E-05    0.11308E-02    0.99887
   27    0.21942E-09    0.51792E-06    0.61518E-03    0.99938

BLOCK:  F-101    MODEL: RSTOIC
------------------------------
  INLET STREAM:            S-220,
  OUTLET STREAM:           S-110
  PROPERTY OPTION SET:     NRTL-RK   RENON (NRTL) / REDLICH-KWONG

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

```
MOLE(LBMOL/HR)          11566.8       10872.5      -694.305       0.00000
MASS(LB/HR   )          290043.       290043.                     0.00000
ENTHALPY(BTU/HR  )   -0.145901E+08 -0.224575E+09                 0.935032

                   ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E              200419.      LB/HR
 PRODUCT STREAMS CO2E           21992.2      LB/HR
 NET STREAMS CO2E PRODUCTION  -178426.      LB/HR
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION        -178426.      LB/HR

                       ***  INPUT DATA  ***
STOICHIOMETRY MATRIX:

 REACTION #   1:
  SUBSTREAM MIXED   :
  METHANE   -1.00    WATER      2.00    OXYGEN    -2.00    CARBO-01   1.00

 REACTION #   2:
  SUBSTREAM MIXED   :
  ETHANE    -2.00    WATER      6.00    OXYGEN    -7.00    CARBO-01   4.00

 REACTION #   3:
  SUBSTREAM MIXED   :
  PROPANE   -1.00    WATER      4.00    OXYGEN    -5.00    CARBO-01   3.00

 REACTION #   4:
  SUBSTREAM MIXED   :
  HYDROGEN  -2.00    WATER      2.00    OXYGEN    -1.00


REACTION CONVERSION SPECS: NUMBER=    4
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:METHANE  CONV FRAC:  1.000
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC:  1.000
  REACTION #   3:
  SUBSTREAM:MIXED    KEY COMP:PROPANE  CONV FRAC:  1.000
  REACTION #   4:
  SUBSTREAM:MIXED    KEY COMP:HYDROGEN CONV FRAC:  1.000



TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                 1,346.00
SPECIFIED PRESSURE    PSIA                                 14.5038
MAXIMUM NO. ITERATIONS                                     30
CONVERGENCE TOLERANCE                                       0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                     1346.0
OUTLET PRESSURE       PSIA                                  14.504
HEAT DUTY             BTU/HR                             -0.20998E+09
VAPOR FRACTION                                              1.0000
```

HEAT OF REACTIONS:

| REACTION NUMBER | REFERENCE COMPONENT | HEAT OF REACTION BTU/LBMOL |
|---|---|---|
| 1 | METHANE | -0.34514E+06 |
| 2 | ETHANE | -0.61431E+06 |
| 3 | PROPANE | -0.87852E+06 |
| 4 | HYDROGEN | -0.10400E+06 |

REACTION EXTENTS:

| REACTION NUMBER | REACTION EXTENT LBMOL/HR |
|---|---|
| 1 | 499.71 |
| 2 | 0.0000 |
| 3 | 0.0000 |
| 4 | 694.31 |

V-L PHASE EQUILIBRIUM :

| COMP | F(I) | X(I) | Y(I) | K(I) |
|---|---|---|---|---|
| WATER | 0.21964 | 0.92206 | 0.21964 | 532.39 |
| OXYGEN | 0.31156E-01 | 0.37057E-02 | 0.31156E-01 | 18791. |
| NITROGEN | 0.70324 | 0.74236E-01 | 0.70324 | 21172. |
| CARBO-01 | 0.45961E-01 | 0.26327E-05 | 0.45961E-01 | 0.39019E+08 |

BLOCK: F-101, MODEL: HEATER
-------------------------------
INLET STREAM: S-106
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) | 23597.0 | 23597.1 | -0.447184E-05 |
| MASS(LB/HR ) | 580599. | 580601. | -0.298171E-05 |
| ENTHALPY(BTU/HR ) | -0.264258E+09 | -0.254505E+09 | -0.369042E-01 |

*** CO2 EQUIVALENT SUMMARY ***

| | | |
|---|---|---|
| FEED STREAMS CO2E | 0.302786E+07 | LB/HR |
| PRODUCT STREAMS CO2E | 0.302790E+07 | LB/HR |
| NET STREAMS CO2E PRODUCTION | 42.0148 | LB/HR |
| UTILITIES CO2E PRODUCTION | 0.00000 | LB/HR |
| TOTAL CO2E PRODUCTION | 42.0148 | LB/HR |

*** INPUT DATA ***

| | | |
|---|---|---|
| TWO PHASE TP FLASH | | |
| SPECIFIED TEMPERATURE | F | 1,166.00 |
| PRESSURE DROP | PSI | 0.0 |
| MAXIMUM NO. ITERATIONS | | 30 |

```
   CONVERGENCE TOLERANCE                                              0.000100000



                        ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                       1166.0
   OUTLET PRESSURE       PSIA                                    43.664
   HEAT DUTY             BTU/HR                                 0.97541E+07
   OUTLET VAPOR FRACTION                                         1.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      HYDROGEN                0.59109E-01       0.43786E-03       0.59109E-01
0.14080E+06
      METHANE          0.31994        0.94192E-01    0.31994        3542.7
      ETHANE           0.55935        0.44805        0.55935        1302.1
      ETHENE           0.34017E-01    0.18588E-01    0.34017E-01    1908.7
      PROPANE          0.14170E-01    0.30878E-01    0.14170E-01    478.63
      PROPENE          0.28474E-02    0.41948E-02    0.28474E-02    707.98
      BENZENE          0.99302E-02    0.35301        0.99302E-02    29.340
      TOLUENE          0.63005E-03    0.50190E-01    0.63005E-03    13.093
      P-XYL-01         0.58145E-05    0.45234E-03    0.58145E-05    13.407
      1:3:5-01         0.39274E-07    0.36109E-05    0.39274E-07    11.344

 BLOCK:  F-401-2  MODEL: RSTOIC
 ------------------------------
   INLET STREAM:          S-221,
   OUTLET STREAM:         S-411
   OUTLET HEAT STREAM:    HEAT1
   PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                               IN             OUT        GENERATION    RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         54270.9       51013.2      -3257.66       0.00000
   MASS(LB/HR   )       0.136087E+07  0.136087E+07                  0.00000
   ENTHALPY(BTU/HR  )   -0.684562E+08 -0.684562E+08                -0.152372E-
14

                   ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            940357.      LB/HR
    PRODUCT STREAMS CO2E         103187.      LB/HR
    NET STREAMS CO2E PRODUCTION  -837171.     LB/HR
    UTILITIES CO2E PRODUCTION     0.00000     LB/HR
    TOTAL CO2E PRODUCTION        -837171.     LB/HR

                       ***  INPUT DATA  ***
   STOICHIOMETRY MATRIX:

    REACTION #   1:
     SUBSTREAM MIXED   :
     METHANE   -1.00    WATER      2.00    OXYGEN    -2.00    CARBO-01   1.00
```

```
 REACTION #   2:
  SUBSTREAM MIXED   :
  HYDROGEN  -2.00    WATER      2.00    OXYGEN    -1.00


REACTION CONVERSION SPECS: NUMBER=    2
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:METHANE  CONV FRAC:  1.000
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:HYDROGEN CONV FRAC:  1.000



TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                  572.000
SPECIFIED PRESSURE    PSIA                                14.5038
MAXIMUM NO. ITERATIONS                                    30
CONVERGENCE TOLERANCE                                      0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES           NO

                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                     572.00
OUTLET PRESSURE       PSIA                                  14.504
HEAT DUTY             BTU/HR                              -0.13050E+10
VAPOR FRACTION                                              1.0000


HEAT OF REACTIONS:

  REACTION          REFERENCE          HEAT OF
  NUMBER            COMPONENT          REACTION
                                        BTU/LBMOL
   1                   METHANE          -0.34514E+06
   2                   HYDROGEN         -0.10400E+06

REACTION EXTENTS:

   REACTION          REACTION
   NUMBER            EXTENT
                     LBMOL/HR
   1                  2344.6
   2                  3257.7

V-L PHASE EQUILIBRIUM :

   COMP              F(I)           X(I)           Y(I)           K(I)
   WATER            0.21964        0.97237        0.21964        67.110
   OXYGEN           0.31156E-01    0.18842E-02    0.31156E-01    4912.9
   NITROGEN         0.70324        0.25672E-01    0.70324        8138.6
   CARBO-01                0.45961E-01       0.72309E-04       0.45961E-01
0.18885E+06

BLOCK:  F-401-2, MODEL: HEATER
------------------------------
```

```
  INLET STREAM:           S-403
  INLET HEAT STREAM:      HEAT1
  OUTLET STREAM:          S-404
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            61691.1         61691.1       -0.353826E-15
      MASS(LB/HR   )           0.111138E+07    0.111138E+07   -0.209497E-15
      ENTHALPY(BTU/HR  )      -0.624944E+10   -0.624944E+10    0.137548E-07

                    ***  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  PQ  FLASH
  SPECIFIED PRESSURE                    PSIA                     464.696
  DUTY FROM INLET HEAT STREAM(S)        BTU/HR                     0.130502+10
  MAXIMUM NO. ITERATIONS                                          30
  CONVERGENCE TOLERANCE                                            0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      465.28
  OUTLET PRESSURE       PSIA                                   464.70
  OUTLET VAPOR FRACTION                                        1.0000



  V-L PHASE EQUILIBRIUM :

     COMP             F(I)           X(I)           Y(I)           K(I)
     WATER            1.0000         1.0000         1.0000         1.0492

BLOCK:  H-101    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             S-107
  OUTLET STREAM:            S-108
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  COLD SIDE:
  ----------
  INLET STREAM:             S-105
  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)            53146.5         53146.5         0.00000
```

```
    MASS(LB/HR   )           0.116120E+07    0.116120E+07     0.00000
    ENTHALPY(BTU/HR  )      -0.788590E+09   -0.788590E+09    0.453503E-15

                  ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E            0.717128E+07  LB/HR
 PRODUCT STREAMS CO2E         0.717128E+07  LB/HR
 NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION         0.00000      LB/HR

                      ***  INPUT DATA  ***

FLASH SPECS FOR HOT SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                     30
CONVERGENCE TOLERANCE                                       0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                     30
CONVERGENCE TOLERANCE                                       0.000100000

FLOW DIRECTION AND SPECIFICATION:
  COUNTERCURRENT   HEAT EXCHANGER
  SPECIFIED COLD APPROACH TEMP
  SPECIFIED VALUE                F                         18.0000
  TEMPERATURE TOLERANCE          F                          0.01800
  LMTD CORRECTION FACTOR                                    1.00000

PRESSURE SPECIFICATION:
  HOT  SIDE PRESSURE DROP        PSI                       10.0000
  COLD SIDE PRESSURE DROP        PSI                       10.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
  HOT LIQUID    COLD LIQUID      BTU/HR-SQFT-R            149.6937
  HOT 2-PHASE   COLD LIQUID      BTU/HR-SQFT-R            149.6937
  HOT VAPOR     COLD LIQUID      BTU/HR-SQFT-R            149.6937
  HOT LIQUID    COLD 2-PHASE     BTU/HR-SQFT-R            149.6937
  HOT 2-PHASE   COLD 2-PHASE     BTU/HR-SQFT-R            149.6937
  HOT VAPOR     COLD 2-PHASE     BTU/HR-SQFT-R            149.6937
  HOT LIQUID    COLD VAPOR       BTU/HR-SQFT-R            149.6937
  HOT 2-PHASE   COLD VAPOR       BTU/HR-SQFT-R            149.6937
  HOT VAPOR     COLD VAPOR       BTU/HR-SQFT-R            149.6937

                    ***  OVERALL RESULTS  ***

STREAMS:
              --------------------------------------
              |                                    |
S-107     ----->|               HOT                |-----> S-108
T=  1.1660D+03  |                                    |         T=
1.0292D+02
P=  3.6412D+01  |                                    |         P=
2.6412D+01
V=  1.0000D+00  |                                    |       V=  9.9275D-
01
              |                                    |
```

```
   S-106     <-----|                COLD                |<----- S-105
   T=  1.1480D+03  |                                    |        T= -
1.7084D+01
   P=  4.3664D+01  |                                      |        P=
5.3664D+01
   V=  1.0000D+00  |                                 |       V=  9.8735D-
01
                   --------------------------------------

   DUTY AND AREA:
     CALCULATED HEAT DUTY          BTU/HR          470058043.9075
     CALCULATED (REQUIRED) AREA    SQFT                60388.0036
     ACTUAL EXCHANGER AREA         SQFT                60388.0036
     PER CENT OVER-DESIGN                                  0.0000

   HEAT TRANSFER COEFFICIENT:
     AVERAGE COEFFICIENT (DIRTY)   BTU/HR-SQFT-R         149.6937
     UA (DIRTY)                    BTU/HR-R          9039701.0442

   LOG-MEAN TEMPERATURE DIFFERENCE:
     LMTD CORRECTION FACTOR                                1.0000
     LMTD (CORRECTED)              F                      51.9993
     NUMBER OF SHELLS IN SERIES                             1

   PRESSURE DROP:
     HOTSIDE, TOTAL                PSI                    10.0000
     COLDSIDE, TOTAL               PSI                    10.0000

                        ***  ZONE RESULTS  ***

   TEMPERATURE LEAVING EACH ZONE:

                                     HOT
         -------------------------------------------------------------
         |                   |                   |                   |
 HOT IN  |        VAP         |        VAP         |        COND        | HOT
OUT
 ------> |                   |                   |                   |------>
 1166.0  |              152.1|              119.9|                   |  102.9
         |                   |                   |                   |
 COLDOUT |       VAP         |       BOIL        |       BOIL        | COLDIN
 <------ |                   |                   |                   |<------
 1148.0  |               41.9|               12.3|                   |  -17.1
         |                   |                   |                   |
         -------------------------------------------------------------
                                     COLD

   ZONE HEAT TRANSFER AND AREA:

   ZONE       HEAT DUTY       AREA       LMTD       AVERAGE U       UA
              BTU/HR          SQFT        F         BTU/HR-SQFT-R   BTU/HR-R
     1  451409557.974     59266.5658     50.8812    149.6937     8871828.9247
     2    9967205.951       611.3995    108.9043    149.6937       91522.6296
     3    8681279.983       510.0382    113.7045    149.6937       76349.4899

 HEATX COLD-TQCU H-101    TQCURV INLET
 -------------------------------------
```

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -10.0000 PSI
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

| DUTY BTU/HR | PRES PSIA | TEMP F | VFRAC |
|---|---|---|---|
| 0.0 | 53.6640 | 1148.0469 | 1.0000 |
| 2.2384+07 | 53.6640 | 1106.3022 | 1.0000 |
| 4.4767+07 | 53.6640 | 1063.9048 | 1.0000 |
| 6.7151+07 | 53.6640 | 1020.8060 | 1.0000 |
| 8.9535+07 | 53.6640 | 976.9512 | 1.0000 |
| 1.1192+08 | 53.6640 | 932.2784 | 1.0000 |
| 1.3430+08 | 53.6640 | 886.7175 | 1.0000 |
| 1.5669+08 | 53.6640 | 840.1877 | 1.0000 |
| 1.7907+08 | 53.6640 | 792.5954 | 1.0000 |
| 2.0145+08 | 53.6640 | 743.8308 | 1.0000 |
| 2.2384+08 | 53.6640 | 693.7630 | 1.0000 |
| 2.4622+08 | 53.6640 | 642.2347 | 1.0000 |
| 2.6860+08 | 53.6640 | 589.0530 | 1.0000 |
| 2.9099+08 | 53.6640 | 533.9787 | 1.0000 |
| 3.1337+08 | 53.6640 | 476.7098 | 1.0000 |
| 3.3576+08 | 53.6640 | 416.8595 | 1.0000 |
| 3.5814+08 | 53.6640 | 353.9281 | 1.0000 |
| 3.8052+08 | 53.6640 | 287.2685 | 1.0000 |
| 4.0291+08 | 53.6640 | 216.0633 | 1.0000 |
| 4.2529+08 | 53.6640 | 139.3669 | 1.0000 |
| 4.4767+08 | 53.6640 | 56.3835 | 1.0000 |
| 4.5136+08 | 53.6640 | 42.1066 | DEW>1.0000 |
| 4.5783+08 | 53.6640 | 23.3187 | 0.9947 |
| 4.7006+08 | 53.6640 | -17.0838 | 0.9874 |

HEATX HOT-TQCUR H-101 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 PSI
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

| DUTY BTU/HR | PRES PSIA | TEMP F | VFRAC |
|---|---|---|---|
| 0.0 | 36.4121 | 1166.0000 | 1.0000 |

```
! 2.2384+07 !    36.4121 !  1125.2901 !     1.0000 !
! 4.4767+07 !    36.4121 !  1084.0343 !     1.0000 !
! 6.7151+07 !    36.4121 !  1042.1961 !     1.0000 !
! 8.9535+07 !    36.4121 !   999.7354 !     1.0000 !
!-----------+------------+------------+------------!
! 1.1192+08 !    36.4121 !   956.6074 !     1.0000 !
! 1.3430+08 !    36.4121 !   912.7621 !     1.0000 !
! 1.5669+08 !    36.4121 !   868.1433 !     1.0000 !
! 1.7907+08 !    36.4121 !   822.6872 !     1.0000 !
! 2.0145+08 !    36.4121 !   776.3206 !     1.0000 !
!-----------+------------+------------+------------!
! 2.2384+08 !    36.4121 !   728.9590 !     1.0000 !
! 2.4622+08 !    36.4121 !   680.5035 !     1.0000 !
! 2.6860+08 !    36.4121 !   630.8374 !     1.0000 !
! 2.9099+08 !    36.4121 !   579.8209 !     1.0000 !
! 3.1337+08 !    36.4121 !   527.2847 !     1.0000 !
!-----------+------------+------------+------------!
! 3.3576+08 !    36.4121 !   473.0211 !     1.0000 !
! 3.5814+08 !    36.4121 !   416.7732 !     1.0000 !
! 3.8052+08 !    36.4121 !   358.2202 !     1.0000 !
! 4.0291+08 !    36.4121 !   296.9623 !     1.0000 !
! 4.2529+08 !    36.4121 !   232.5095 !     1.0000 !
!-----------+------------+------------+------------!
! 4.4767+08 !    36.4121 !   164.2910 !     1.0000 !
! 4.5136+08 !    36.4121 !   152.6582 !     1.0000 !
! 4.5783+08 !    36.4121 !   131.9430 ! DEW>1.0000 !
! 4.7006+08 !    36.4121 !   108.6945 !     0.9891 !
-----------------------------------------------------

BLOCK:  H-201    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             S-314
  OUTLET STREAM:            S-215
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  COLD SIDE:
  ----------
  INLET STREAM:             S-211
  OUTLET STREAM:            S-212
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            28877.9         28877.9          0.00000
      MASS(LB/HR   )            547777.         547777.          0.00000
      ENTHALPY(BTU/HR  )      -0.529803E+09   -0.529803E+09     0.00000

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.407420E+07  LB/HR
   PRODUCT STREAMS CO2E         0.407420E+07  LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                         ***  INPUT DATA  ***
```

```
   FLASH SPECS FOR HOT SIDE:
   TWO    PHASE      FLASH
   MAXIMUM NO. ITERATIONS                                      30
   CONVERGENCE TOLERANCE                                        0.000100000

   FLASH SPECS FOR COLD SIDE:
   TWO    PHASE      FLASH
   MAXIMUM NO. ITERATIONS                                      30
   CONVERGENCE TOLERANCE                                        0.000100000

   FLOW DIRECTION AND SPECIFICATION:
     COUNTERCURRENT   HEAT EXCHANGER
     SPECIFIED HOT APPROACH TEMP
     SPECIFIED VALUE                 F                         32.4000
     TEMPERATURE TOLERANCE           F                          0.01800
     LMTD CORRECTION FACTOR                                     1.00000

   PRESSURE SPECIFICATION:
     HOT  SIDE PRESSURE DROP         PSI                       10.0000
     COLD SIDE PRESSURE DROP         PSI                       10.0000

   HEAT TRANSFER COEFFICIENT SPECIFICATION:
     HOT LIQUID    COLD LIQUID      BTU/HR-SQFT-R             149.6937
     HOT 2-PHASE   COLD LIQUID      BTU/HR-SQFT-R             149.6937
     HOT VAPOR     COLD LIQUID      BTU/HR-SQFT-R             149.6937
     HOT LIQUID    COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
     HOT 2-PHASE   COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
     HOT VAPOR     COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
     HOT LIQUID    COLD VAPOR       BTU/HR-SQFT-R             149.6937
     HOT 2-PHASE   COLD VAPOR       BTU/HR-SQFT-R             149.6937
     HOT VAPOR     COLD VAPOR       BTU/HR-SQFT-R             149.6937

                     ***  OVERALL RESULTS  ***

   STREAMS:
                    --------------------------------------
                    |                                    |
   S-314     ----->|                HOT                 |-----> S-215
   T=   2.4971D+02  |                                    |         T=
1.3640D+02
   P=   3.5000D+01  |                                    |         P=
2.5000D+01
   V=   0.0000D+00  |                                    |         V=
0.0000D+00
                    |                                    |
   S-212     <-----|                COLD                |<----- S-211
   T=   1.2634D+02  |                                    |         T=
1.0400D+02
   P=   7.2000D+02  |                                    |         P=
7.3000D+02
   V=   1.0000D+00  |                                    |         V=
1.0000D+00
                    --------------------------------------

   DUTY AND AREA:
     CALCULATED HEAT DUTY            BTU/HR               6478222.0023
```

```
    CALCULATED (REQUIRED) AREA     SQFT                      636.0483
    ACTUAL EXCHANGER AREA          SQFT                      636.0483
    PER CENT OVER-DESIGN                                       0.0000

  HEAT TRANSFER COEFFICIENT:
    AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R             149.6937
    UA (DIRTY)                     BTU/HR-R                95212.3982

  LOG-MEAN TEMPERATURE DIFFERENCE:
    LMTD CORRECTION FACTOR                                     1.0000
    LMTD (CORRECTED)               F                          68.0397
    NUMBER OF SHELLS IN SERIES                                   1

  PRESSURE DROP:
    HOTSIDE, TOTAL                 PSI                        10.0000
    COLDSIDE, TOTAL                PSI                        10.0000

                      ***  ZONE RESULTS  ***

  TEMPERATURE LEAVING EACH ZONE:

                                   HOT
         -------------------------------------------------------------
         |                                                           |
 HOT IN  |                           LIQ                                | HOT
OUT
 ------> |                                                           |------>
  249.7  |                                                           |  136.4
         |                                                           |
 COLDOUT |                         VAP                               | COLDIN
 <------ |                                                           |<------
  126.3  |                                                           |  104.0
         |                                                           |
         -------------------------------------------------------------
                                   COLD

  ZONE HEAT TRANSFER AND AREA:

  ZONE       HEAT DUTY        AREA       LMTD       AVERAGE U       UA
             BTU/HR           SQFT        F         BTU/HR-SQFT-R   BTU/HR-R
    1    6478222.002       636.0483      68.0397   149.6937       95212.3982

 HEATX COLD-TQCU H-201    TQCURV INLET
 -------------------------------------
  PRESSURE PROFILE:      CONSTANT2
  PRESSURE DROP:         -10.0000    PSI
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

 -----------------------------------------------------
 !  DUTY       !  PRES       !  TEMP       !  VFRAC      !
 !             !             !             !             !
 !             !             !             !             !
 !             !             !             !             !
 !  BTU/HR     !  PSIA       !  F          !             !
 !             !             !             !             !
 !============!============!============!============!
 !     0.0     !   729.9998 !   126.6736 !     1.0000 !
```

```
!  3.0849+05 !   729.9998 !   125.5962 !     1.0000 !
!  6.1697+05 !   729.9998 !   124.5186 !     1.0000 !
!  9.2546+05 !   729.9998 !   123.4407 !     1.0000 !
!  1.2339+06 !   729.9998 !   122.3625 !     1.0000 !
!------------+------------+------------+------------!
!  1.5424+06 !   729.9998 !   121.2841 !     1.0000 !
!  1.8509+06 !   729.9998 !   120.2054 !     1.0000 !
!  2.1594+06 !   729.9998 !   119.1265 !     1.0000 !
!  2.4679+06 !   729.9998 !   118.0474 !     1.0000 !
!  2.7764+06 !   729.9998 !   116.9680 !     1.0000 !
!------------+------------+------------+------------!
!  3.0849+06 !   729.9998 !   115.8884 !     1.0000 !
!  3.3934+06 !   729.9998 !   114.8086 !     1.0000 !
!  3.7018+06 !   729.9998 !   113.7286 !     1.0000 !
!  4.0103+06 !   729.9998 !   112.6484 !     1.0000 !
!  4.3188+06 !   729.9998 !   111.5680 !     1.0000 !
!------------+------------+------------+------------!
!  4.6273+06 !   729.9998 !   110.4874 !     1.0000 !
!  4.9358+06 !   729.9998 !   109.4066 !     1.0000 !
!  5.2443+06 !   729.9998 !   108.3257 !     1.0000 !
!  5.5528+06 !   729.9998 !   107.2445 !     1.0000 !
!  5.8612+06 !   729.9998 !   106.1633 !     1.0000 !
!------------+------------+------------+------------!
!  6.1697+06 !   729.9998 !   105.0819 !     1.0000 !
!  6.4782+06 !   729.9998 !   103.9998 !     1.0000 !
-----------------------------------------------------

HEATX HOT-TQCUR H-201    TQCURV INLET
-------------------------------------
  PRESSURE PROFILE:      CONSTANT2
  PRESSURE DROP:         0.0          PSI
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

-----------------------------------------------------
!  DUTY      !  PRES      !  TEMP      !  VFRAC     !
!            !            !            !            !
!            !            !            !            !
!            !            !            !            !
!  BTU/HR    !  PSIA      !  F         !            !
!            !            !            !            !
!============!============!============!============!
!     0.0    !    35.0000 !   249.7144 !     0.0    !
!  3.0849+05 !    35.0000 !   244.5803 !     0.0    !
!  6.1697+05 !    35.0000 !   239.4215 !     0.0    !
!  9.2546+05 !    35.0000 !   234.2379 !     0.0    !
!  1.2339+06 !    35.0000 !   229.0292 !     0.0    !
!------------+------------+------------+------------!
!  1.5424+06 !    35.0000 !   223.7951 !     0.0    !
!  1.8509+06 !    35.0000 !   218.5355 !     0.0    !
!  2.1594+06 !    35.0000 !   213.2499 !     0.0    !
!  2.4679+06 !    35.0000 !   207.9382 !     0.0    !
!  2.7764+06 !    35.0000 !   202.6000 !     0.0    !
!------------+------------+------------+------------!
!  3.0849+06 !    35.0000 !   197.2351 !     0.0    !
!  3.3934+06 !    35.0000 !   191.8430 !     0.0    !
!  3.7018+06 !    35.0000 !   186.4235 !     0.0    !
!  4.0103+06 !    35.0000 !   180.9762 !     0.0    !
```

```
!  4.3188+06 !    35.0000 !   175.5008 !     0.0    !
!------------+------------+------------+------------!
!  4.6273+06 !    35.0000 !   169.9968 !     0.0    !
!  4.9358+06 !    35.0000 !   164.4640 !     0.0    !
!  5.2443+06 !    35.0000 !   158.9019 !     0.0    !
!  5.5528+06 !    35.0000 !   153.3102 !     0.0    !
!  5.8612+06 !    35.0000 !   147.6886 !     0.0    !
!------------+------------+------------+------------!
!  6.1697+06 !    35.0000 !   142.0365 !     0.0    !
!  6.4782+06 !    35.0000 !   136.3537 !     0.0    !
-----------------------------------------------------

BLOCK:  H-202    MODEL: HEATX
-----------------------------
  HOT SIDE:
  ---------
  INLET STREAM:             S-318
  OUTLET STREAM:            S-216
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
  COLD SIDE:
  ----------
  INLET STREAM:             S-212
  OUTLET STREAM:            S-213
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           27588.5         27588.5         0.00000
      MASS(LB/HR   )           443383.         443383.         0.00000
      ENTHALPY(BTU/HR  )     -0.554466E+09   -0.554466E+09     0.00000

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E           0.407420E+07  LB/HR
   PRODUCT STREAMS CO2E        0.407420E+07  LB/HR
   NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
   UTILITIES CO2E PRODUCTION     0.00000      LB/HR
   TOTAL CO2E PRODUCTION         0.00000      LB/HR

                         ***  INPUT DATA  ***

  FLASH SPECS FOR HOT SIDE:
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                 30
  CONVERGENCE TOLERANCE                                   0.000100000

  FLASH SPECS FOR COLD SIDE:
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                 30
  CONVERGENCE TOLERANCE                                   0.000100000

  FLOW DIRECTION AND SPECIFICATION:
    COUNTERCURRENT   HEAT EXCHANGER
    SPECIFIED HOT APPROACH TEMP
    SPECIFIED VALUE                F                     18.0000
    TEMPERATURE TOLERANCE          F                      0.01800
    LMTD CORRECTION FACTOR                                1.00000
```

```
PRESSURE SPECIFICATION:
  HOT  SIDE PRESSURE DROP        PSI                        10.0000
  COLD SIDE PRESSURE DROP        PSI                        10.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
  HOT LIQUID    COLD LIQUID      BTU/HR-SQFT-R             149.6937
  HOT 2-PHASE   COLD LIQUID      BTU/HR-SQFT-R             149.6937
  HOT VAPOR     COLD LIQUID      BTU/HR-SQFT-R             149.6937
  HOT LIQUID    COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
  HOT 2-PHASE   COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
  HOT VAPOR     COLD 2-PHASE     BTU/HR-SQFT-R             149.6937
  HOT LIQUID    COLD VAPOR       BTU/HR-SQFT-R             149.6937
  HOT 2-PHASE   COLD VAPOR       BTU/HR-SQFT-R             149.6937
  HOT VAPOR     COLD VAPOR       BTU/HR-SQFT-R             149.6937

                     ***  OVERALL RESULTS  ***

STREAMS:
                --------------------------------------
                |                                    |
S-318     ----->|                HOT                 |-----> S-216
T=   3.2379D+02  |                                    |         T=
1.4434D+02
P=   1.3750D+01  |                                    |         P=
3.7500D+00
V=   0.0000D+00  |                                    |         V=
0.0000D+00
                |                                    |
S-213     <-----|                COLD                |<----- S-212
T=   1.2963D+02  |                                    |         T=
1.2634D+02
P=   7.1000D+02  |                                    |         P=
7.2000D+02
V=   1.0000D+00  |                                    |         V=
1.0000D+00
                --------------------------------------

DUTY AND AREA:
  CALCULATED HEAT DUTY           BTU/HR                1034205.0395
  CALCULATED (REQUIRED) AREA     SQFT                       93.2750
  ACTUAL EXCHANGER AREA          SQFT                       93.2750
  PER CENT OVER-DESIGN                                       0.0000

HEAT TRANSFER COEFFICIENT:
  AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R             149.6937
  UA (DIRTY)                     BTU/HR-R                13962.6760

LOG-MEAN TEMPERATURE DIFFERENCE:
  LMTD CORRECTION FACTOR                                     1.0000
  LMTD (CORRECTED)               F                          74.0693
  NUMBER OF SHELLS IN SERIES                                1

PRESSURE DROP:
  HOTSIDE, TOTAL                 PSI                        10.0000
  COLDSIDE, TOTAL                PSI                        10.0000
```

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

```
                                    HOT
        -------------------------------------------------------------
        |                                                           |
 HOT IN |                             LIQ                               | HOT
OUT
 ------> |                                                          |------>
  323.8  |                                                          |  144.3
        |                                                           |
 COLDOUT |                            VAP                           | COLDIN
 <------ |                                                          |<------
  129.6  |                                                          |  126.3
        |                                                           |
        -------------------------------------------------------------
                                    COLD
```

ZONE HEAT TRANSFER AND AREA:

| ZONE | HEAT DUTY<br>BTU/HR | AREA<br>SQFT | LMTD<br>F | AVERAGE U<br>BTU/HR-SQFT-R | UA<br>BTU/HR-R |
|---|---|---|---|---|---|
| 1 | 1034205.039 | 93.2750 | 74.0693 | 149.6937 | 13962.6760 |

HEATX COLD-TQCU H-202 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: -10.0000 PSI
PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

| DUTY<br>BTU/HR | PRES<br>PSIA | TEMP<br>F | VFRAC |
|---|---|---|---|
| 0.0 | 719.9998 | 129.9567 | 1.0000 |
| 4.9248+04 | 719.9998 | 129.7847 | 1.0000 |
| 9.8496+04 | 719.9998 | 129.6126 | 1.0000 |
| 1.4774+05 | 719.9998 | 129.4406 | 1.0000 |
| 1.9699+05 | 719.9998 | 129.2685 | 1.0000 |
| 2.4624+05 | 719.9998 | 129.0964 | 1.0000 |
| 2.9549+05 | 719.9998 | 128.9243 | 1.0000 |
| 3.4474+05 | 719.9998 | 128.7522 | 1.0000 |
| 3.9398+05 | 719.9998 | 128.5801 | 1.0000 |
| 4.4323+05 | 719.9998 | 128.4080 | 1.0000 |
| 4.9248+05 | 719.9998 | 128.2359 | 1.0000 |
| 5.4173+05 | 719.9998 | 128.0638 | 1.0000 |
| 5.9097+05 | 719.9998 | 127.8916 | 1.0000 |
| 6.4022+05 | 719.9998 | 127.7195 | 1.0000 |
| 6.8947+05 | 719.9998 | 127.5473 | 1.0000 |

| | | | |
|---|---|---|---|
| 7.3872+05 | 719.9998 | 127.3752 | 1.0000 |
| 7.8797+05 | 719.9998 | 127.2030 | 1.0000 |
| 8.3721+05 | 719.9998 | 127.0308 | 1.0000 |
| 8.8646+05 | 719.9998 | 126.8587 | 1.0000 |
| 9.3571+05 | 719.9998 | 126.6865 | 1.0000 |
| 9.8496+05 | 719.9998 | 126.5143 | 1.0000 |
| 1.0342+06 | 719.9998 | 126.3421 | 1.0000 |

HEATX HOT-TQCUR H-202    TQCURV INLET

PRESSURE PROFILE:      CONSTANT2
PRESSURE DROP:         0.0         PSI
PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

| DUTY BTU/HR | PRES PSIA | TEMP F | VFRAC |
|---|---|---|---|
| 0.0 | 13.7500 | 323.7883 | 0.0 |
| 4.9248+04 | 13.7500 | 315.9888 | 0.0 |
| 9.8496+04 | 13.7500 | 308.1228 | 0.0 |
| 1.4774+05 | 13.7500 | 300.1892 | 0.0 |
| 1.9699+05 | 13.7500 | 292.1869 | 0.0 |
| 2.4624+05 | 13.7500 | 284.1147 | 0.0 |
| 2.9549+05 | 13.7500 | 275.9711 | 0.0 |
| 3.4474+05 | 13.7500 | 267.7550 | 0.0 |
| 3.9398+05 | 13.7500 | 259.4649 | 0.0 |
| 4.4323+05 | 13.7500 | 251.0994 | 0.0 |
| 4.9248+05 | 13.7500 | 242.6569 | 0.0 |
| 5.4173+05 | 13.7500 | 234.1361 | 0.0 |
| 5.9097+05 | 13.7500 | 225.5354 | 0.0 |
| 6.4022+05 | 13.7500 | 216.8533 | 0.0 |
| 6.8947+05 | 13.7500 | 208.0882 | 0.0 |
| 7.3872+05 | 13.7500 | 199.2386 | 0.0 |
| 7.8797+05 | 13.7500 | 190.3031 | 0.0 |
| 8.3721+05 | 13.7500 | 181.2802 | 0.0 |
| 8.8646+05 | 13.7500 | 172.1684 | 0.0 |
| 9.3571+05 | 13.7500 | 162.9666 | 0.0 |
| 9.8496+05 | 13.7500 | 153.6736 | 0.0 |
| 1.0342+06 | 13.7500 | 144.2882 | 0.0 |

BLOCK:  H-203    MODEL: HEATER

INLET STREAM:          S-213
OUTLET STREAM:         S-214
OUTLET HEAT STREAM:    HEAT2

```
PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
 TOTAL BALANCE
    MOLE(LBMOL/HR)            27489.1          27489.1         0.00000
    MASS(LB/HR   )            431442.          431442.         0.00000
    ENTHALPY(BTU/HR  )      -0.552102E+09   -0.552102E+09     0.00000

                   ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E            0.407420E+07  LB/HR
 PRODUCT STREAMS CO2E         0.407420E+07  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                          181.400
PRESSURE DROP                      PSI                         10.0000
MAXIMUM NO. ITERATIONS                                         30
CONVERGENCE TOLERANCE                                           0.000100000



                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                    181.40
OUTLET PRESSURE       PSIA                                 700.00
HEAT DUTY             BTU/HR                              0.15007E+08
OUTLET VAPOR FRACTION                                      1.0000



V-L PHASE EQUILIBRIUM :

   COMP              F(I)           X(I)            Y(I)           K(I)
   HYDROGEN                0.33827               0.47059E-06       0.33827
0.14976E+07
   METHANE          0.36954        0.21974        0.36954         3.5036
   ETHANE           0.24974        0.45435        0.24974         1.1452
   ETHENE           0.28397E-01    0.44096E-01    0.28397E-01     1.3417
   PROPANE          0.69941E-02    0.22279E-01    0.69941E-02    0.65404
   PROPENE          0.23182E-02    0.58043E-02    0.23182E-02    0.83209
   BENZENE           0.45756E-02    0.23448         0.45756E-02    0.40654E-
01
   TOLUENE           0.16047E-03    0.18875E-01    0.16047E-03    0.17712E-
01
   P-XYL-01          0.13010E-05    0.34907E-03    0.13010E-05    0.77647E-
02
   1:3:5-01          0.33706E-07    0.20497E-04    0.33706E-07    0.34261E-
02

 BLOCK:  H-203,   MODEL: HEATER
 ------------------------------
  INLET STREAM:           S-407
  INLET HEAT STREAM:      HEAT2
  OUTLET STREAM:          S-217
```

```
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           1073.43         1073.43         0.00000
      MASS(LB/HR   )           19338.1         19338.1         0.00000
      ENTHALPY(BTU/HR  )     -0.124843E+09   -0.124843E+09     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  ***
  TWO    PHASE  PQ  FLASH
  PRESSURE DROP                        PSI                        10.0000
  DUTY FROM INLET HEAT STREAM(S)       BTU/HR                     -0.150066+08
  MAXIMUM NO. ITERATIONS                                          30
  CONVERGENCE TOLERANCE                                            0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      380.29
  OUTLET PRESSURE       PSIA                                   196.00
  OUTLET VAPOR FRACTION                                       0.42023E-01



  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)          K(I)
     WATER             1.0000        1.0000        1.0000        1.0000

BLOCK:  P-201    MODEL: PUMP
----------------------------
  INLET STREAM:           S-204
  OUTLET STREAM:          S-209
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           723.567         723.567         0.00000
      MASS(LB/HR   )           62886.0         62886.0        0.115701E-15
      ENTHALPY(BTU/HR  )      0.355826E+07    0.355047E+07    0.218946E-02

                    ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            6188.99      LB/HR
   PRODUCT STREAMS CO2E         6188.99      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                                  11.8000
   PUMP EFFICIENCY                                         0.80000
   DRIVER EFFICIENCY                                       1.00000

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

                       ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                        1,215.18
   PRESSURE CHANGE  PSI                                   -43.3066
   NPSH AVAILABLE   FT-LBF/LB                              0.0
   FLUID POWER  HP                                        -3.82731
   BRAKE POWER  HP                                        -3.06185
   ELECTRICITY  KW                                        -2.28322
   PUMP EFFICIENCY USED                                    0.80000
   NET WORK REQUIRED  HP                                  -3.06185
   HEAD DEVELOPED FT-LBF/LB                             -120.505

BLOCK:  P-401    MODEL: PUMP
----------------------------
  INLET STREAM:          S-401
  OUTLET STREAM:         S-402
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          57897.2         57897.2         0.00000
      MASS(LB/HR   )        0.104303E+07    0.104303E+07     0.00000
      ENTHALPY(BTU/HR  )   -0.711397E+10   -0.711322E+10   -0.104463E-03

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

                      ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                 205.632
   PUMP EFFICIENCY                                         0.80000
   DRIVER EFFICIENCY                                       1.00000

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

                       ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                       16,809.4
   PRESSURE CHANGE  PSI                                  191.128
   NPSH AVAILABLE   FT-LBF/LB                             32.5915
```

```
  FLUID POWER  HP                                           233.654
  BRAKE POWER  HP                                           292.067
  ELECTRICITY  KW                                           217.795
  PUMP EFFICIENCY USED                                        0.80000
  NET WORK REQUIRED  HP                                     292.067
  HEAD DEVELOPED FT-LBF/LB                                  443.547

BLOCK:  PR-201   MODEL: SEP
---------------------------
 INLET STREAM:          S-214
 OUTLET STREAMS:        S-219,      S-218
 PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)            27489.1         27489.1         0.00000
     MASS(LB/HR   )            431442.         431442.       -0.269828E-15
     ENTHALPY(BTU/HR  )      -0.537095E+09   -0.539039E+09    0.360651E-02

                    ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E            0.407420E+07  LB/HR
  PRODUCT STREAMS CO2E         0.407420E+07  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  ***

 INLET PRESSURE DROP   PSI                                   10.0000

 FLASH SPECS FOR STREAM S-219,
 TWO    PHASE  TP  FLASH
 PRESSURE DROP         PSI                                    0.0
 MAXIMUM NO. ITERATIONS                                      30
 CONVERGENCE TOLERANCE                                        0.000100000

 FLASH SPECS FOR STREAM S-218
 TWO    PHASE  TP  FLASH
 PRESSURE DROP         PSI                                    0.0
 MAXIMUM NO. ITERATIONS                                      30
 CONVERGENCE TOLERANCE                                        0.000100000

 FRACTION OF FEED
   SUBSTREAM= MIXED
     STREAM= S-219,    CPT= HYDROGEN  FRACTION=          0.85000
                            METHANE                      0.28000
                            ETHANE                       0.0
                            ETHENE                       0.0
                            PROPANE                      0.0
                            PROPENE                      0.0
                            BENZENE                      0.0
                            TOLUENE                      0.0
                            P-XYL-01                     0.0
                            1:3:5-01                     0.0
                            WATER                        0.0
```

```
                               OXYGEN                      0.0
                               NITROGEN                    0.0
                               CARBO-01                    0.0


                             ***  RESULTS  ***

  HEAT DUTY             BTU/HR                               -0.19441E+07

 COMPONENT = HYDROGEN
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-219,     MIXED                 0.85000
   S-218      MIXED                 0.15000

 COMPONENT = METHANE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-219,     MIXED                 0.28000
   S-218      MIXED                 0.72000

 COMPONENT = ETHANE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = ETHENE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = PROPANE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = PROPENE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = BENZENE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = TOLUENE
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = P-XYL-01
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

 COMPONENT = 1:3:5-01
   STREAM     SUBSTREAM    SPLIT FRACTION
   S-218      MIXED                 1.00000

BLOCK:  PR-201,  MODEL: VALVE
-----------------------------
  INLET STREAM:          S-219,
  OUTLET STREAM:         S-219
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG
```

```
                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           10748.3         10748.3         0.00000
       MASS(LB/HR   )           61564.4         61564.4         0.00000
       ENTHALPY(BTU/HR  )     -0.828870E+08   -0.828870E+08     0.00000

                    ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.114078E+07  LB/HR
    PRODUCT STREAMS CO2E          0.114078E+07  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                          200.000
    VALVE FLOW COEF CALC.                                   NO

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

                        ***  RESULTS  ***

    VALVE PRESSURE DROP       PSI                           490.000

 BLOCK:  R-101    MODEL: RSTOIC
 ------------------------------
   INLET STREAM:           S-106,
   OUTLET STREAM:          S-107
   PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                           IN             OUT         GENERATION    RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         23597.1       29549.4       5952.29      0.123115E-
15
   MASS(LB/HR   )         580601.       580601.                    0.200508E-
15
   ENTHALPY(BTU/HR  )   -0.254505E+09 -0.542745E+08               -0.786745

                    ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E             0.302790E+07  LB/HR
    PRODUCT STREAMS CO2E          0.414343E+07  LB/HR
    NET STREAMS CO2E PRODUCTION   0.111552E+07  LB/HR
    UTILITIES CO2E PRODUCTION      0.00000      LB/HR
    TOTAL CO2E PRODUCTION         0.111552E+07  LB/HR

                        ***  INPUT DATA  ***
   STOICHIOMETRY MATRIX:

    REACTION #   1:
     SUBSTREAM MIXED   :
     HYDROGEN  -1.00    METHANE    2.00    ETHANE    -1.00
```

```
REACTION #   2:
 SUBSTREAM MIXED   :
 HYDROGEN   1.00    ETHANE    -1.00    ETHENE     1.00

REACTION #   3:
 SUBSTREAM MIXED   :
 HYDROGEN   3.00    ETHANE    -3.00    PROPENE    2.00

REACTION #   4:
 SUBSTREAM MIXED   :
 HYDROGEN   1.00    ETHANE    -3.00    PROPANE    2.00

REACTION #   5:
 SUBSTREAM MIXED   :
 HYDROGEN   6.00    ETHANE    -3.00    BENZENE    1.00

REACTION #   6:
 SUBSTREAM MIXED   :
 HYDROGEN   6.00    METHANE    1.00    ETHANE    -4.00    TOLUENE    1.00

REACTION #   7:
 SUBSTREAM MIXED   :
 HYDROGEN   7.00    ETHANE    -4.00    P-XYL-01   1.00

REACTION #   8:
 SUBSTREAM MIXED   :
 HYDROGEN   7.00    METHANE    1.00    ETHANE    -5.00    1:3:5-01   1.00

REACTION #   9:
 SUBSTREAM MIXED   :
 HYDROGEN  -2.00    METHANE    2.00    ETHENE    -1.00

REACTION #  10:
 SUBSTREAM MIXED   :
 ETHENE    -3.00    PROPENE    2.00

REACTION #  11:
 SUBSTREAM MIXED   :
 HYDROGEN  -2.00    ETHENE    -3.00    PROPANE    2.00

REACTION #  12:
 SUBSTREAM MIXED   :
 HYDROGEN   3.00    ETHENE    -3.00    BENZENE    1.00

REACTION #  13:
 SUBSTREAM MIXED   :
 HYDROGEN   2.00    METHANE    1.00    ETHENE    -4.00    TOLUENE    1.00

REACTION #  14:
 SUBSTREAM MIXED   :
 HYDROGEN   3.00    ETHENE    -4.00    P-XYL-01   1.00

REACTION #  15:
 SUBSTREAM MIXED   :
 HYDROGEN   2.00    METHANE    1.00    ETHENE    -5.00    1:3:5-01   1.00
```

```
 REACTION #  16:
  SUBSTREAM MIXED   :
  HYDROGEN   5.00    PROPANE   -2.00    BENZENE    1.00

 REACTION #  17:
  SUBSTREAM MIXED   :
  HYDROGEN   5.00    ETHANE     1.00    PROPANE   -3.00    TOLUENE    1.00

 REACTION #  18:
  SUBSTREAM MIXED   :
  HYDROGEN   5.00    METHANE    1.00    PROPANE   -3.00    P-XYL-01   1.00

 REACTION #  19:
  SUBSTREAM MIXED   :
  HYDROGEN  -1.00    METHANE    1.00    ETHENE     1.00    PROPENE   -1.00

 REACTION #  20:
  SUBSTREAM MIXED   :
  HYDROGEN   3.00    PROPENE   -2.00    BENZENE    1.00

 REACTION #  21:
  SUBSTREAM MIXED   :
  HYDROGEN   2.00    ETHANE     1.00    PROPENE   -3.00    TOLUENE    1.00

 REACTION #  22:
  SUBSTREAM MIXED   :
  HYDROGEN   2.00    METHANE    1.00    PROPENE   -3.00    P-XYL-01   1.00

 REACTION #  23:
  SUBSTREAM MIXED   :
  HYDROGEN   6.00    PROPANE   -3.00    1:3:5-01   1.00

 REACTION #  24:
  SUBSTREAM MIXED   :
  HYDROGEN   3.00    PROPENE   -3.00    1:3:5-01   1.00


REACTION CONVERSION SPECS: NUMBER=   24
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.7582E-01
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.5904E-01
  REACTION #   3:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.7180E-02
  REACTION #   4:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.6850E-02
  REACTION #   5:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.1737
  REACTION #   6:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.9250E-01
  REACTION #   7:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.1934E-01
  REACTION #   8:
  SUBSTREAM:MIXED    KEY COMP:ETHANE   CONV FRAC: 0.2982E-01
  REACTION #   9:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.1871
  REACTION #  10:
```

```
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.1770E-01
  REACTION #  11:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.1690E-01
  REACTION #  12:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.4287
  REACTION #  13:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.2283
  REACTION #  14:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.4770E-01
  REACTION #  15:
  SUBSTREAM:MIXED    KEY COMP:ETHENE   CONV FRAC: 0.7360E-01
  REACTION #  16:
  SUBSTREAM:MIXED    KEY COMP:PROPANE  CONV FRAC: 0.1815
  REACTION #  17:
  SUBSTREAM:MIXED    KEY COMP:PROPANE  CONV FRAC: 0.2333
  REACTION #  18:
  SUBSTREAM:MIXED    KEY COMP:PROPANE  CONV FRAC: 0.1037
  REACTION #  19:
  SUBSTREAM:MIXED    KEY COMP:PROPENE  CONV FRAC: 0.3487
  REACTION #  20:
  SUBSTREAM:MIXED    KEY COMP:PROPENE  CONV FRAC: 0.2280
  REACTION #  21:
  SUBSTREAM:MIXED    KEY COMP:PROPENE  CONV FRAC: 0.2931
  REACTION #  22:
  SUBSTREAM:MIXED    KEY COMP:PROPENE  CONV FRAC: 0.1303
  REACTION #  23:
  SUBSTREAM:MIXED    KEY COMP:PROPANE  CONV FRAC: 0.6466E-01
  REACTION #  24:
  SUBSTREAM:MIXED    KEY COMP:PROPENE  CONV FRAC: 0.8119E-01


TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                                  1,166.00
PRESSURE DROP         PSI                                    7.25189
MAXIMUM NO. ITERATIONS                                     30
CONVERGENCE TOLERANCE                                       0.000100000
SIMULTANEOUS REACTIONS
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                        ***  RESULTS  ***
OUTLET TEMPERATURE    F                                      1166.0
OUTLET PRESSURE       PSIA                                   36.412
HEAT DUTY             BTU/HR                                0.20023E+09
VAPOR FRACTION                                               1.0000


HEAT OF REACTIONS:

  REACTION          REFERENCE          HEAT OF
  NUMBER            COMPONENT          REACTION
                                        BTU/LBMOL
   1                   ETHANE            -31236.
   2                   ETHANE             61556.
   3                   ETHANE             44994.
```

| | | |
|---|---|---|
| 4 | ETHANE | 7607.0 |
| 5 | ETHANE | 53804. |
| 6 | ETHANE | 37863. |
| 7 | ETHANE | 43254. |
| 8 | ETHANE | 32513. |
| 9 | ETHENE | -92791. |
| 10 | ETHENE | -16563. |
| 11 | ETHENE | -53951. |
| 12 | ETHENE | -7751.3 |
| 13 | ETHENE | -23693. |
| 14 | ETHENE | -18302. |
| 15 | ETHENE | -29043. |
| 16 | PROPANE | 69298. |
| 17 | PROPANE | 44281. |
| 18 | PROPANE | 41058. |
| 19 | PROPENE | -21553. |
| 20 | PROPENE | 13218. |
| 21 | PROPENE | -11800. |
| 22 | PROPENE | -15023. |
| 23 | PROPANE | 47987. |
| 24 | PROPENE | -8094.4 |

REACTION EXTENTS:

| REACTION NUMBER | REACTION EXTENT LBMOL/HR |
|---|---|
| 1 | 1000.8 |
| 2 | 779.28 |
| 3 | 31.590 |
| 4 | 30.138 |
| 5 | 764.32 |
| 6 | 305.23 |
| 7 | 63.818 |
| 8 | 78.720 |
| 9 | 150.19 |
| 10 | 4.7360 |
| 11 | 4.5219 |
| 12 | 114.71 |
| 13 | 45.815 |
| 14 | 9.5723 |
| 15 | 11.816 |
| 16 | 30.349 |
| 17 | 26.003 |
| 18 | 11.558 |
| 19 | 23.429 |
| 20 | 7.6597 |
| 21 | 6.5645 |
| 22 | 2.9183 |
| 23 | 7.2063 |
| 24 | 1.8184 |

V-L PHASE EQUILIBRIUM :

| COMP | F(I) | X(I) | Y(I) | K(I) |
|---|---|---|---|---|
| HYDROGEN | 0.31468 | 0.64800E-03 | 0.31468 | 0.17991E+06 |

```
    METHANE          0.34962        0.28630E-01    0.34962         4524.0
    ETHANE           0.24040        0.53596E-01    0.24040         1661.7
    ETHENE           0.27165E-01    0.41307E-02    0.27165E-01     2436.3
    PROPANE          0.70624E-02    0.42859E-02    0.70624E-02     610.46
    PROPENE          0.22738E-02    0.89976E-03    0.22738E-02     936.21
    BENZENE          0.38964E-01    0.44949        0.38964E-01     32.113
    TOLUENE          0.13485E-01    0.30494        0.13485E-01     16.383
    P-XYL-01         0.29782E-02    0.66877E-01    0.29782E-02     16.498
    1:3:5-01         0.33693E-02    0.86506E-01    0.33693E-02     14.429

BLOCK:  RB-301   MODEL: HEATER
------------------------------
  INLET STREAM:           S-408
  INLET HEAT STREAM:      HEAT3
  OUTLET STREAM:          S-308
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            646.083         646.083         0.00000
      MASS(LB/HR   )            11639.4         11639.4         0.00000
      ENTHALPY(BTU/HR  )      -0.751412E+08   -0.751412E+08    0.198309E-15

                    ***  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  PQ  FLASH
  PRESSURE DROP                         PSI                       10.0000
  DUTY FROM INLET HEAT STREAM(S)        BTU/HR            -9,032,280.
  MAXIMUM NO. ITERATIONS                                          30
  CONVERGENCE TOLERANCE                                            0.000100000



                         ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     380.29
  OUTLET PRESSURE       PSIA                                  196.00
  OUTLET VAPOR FRACTION                                      0.42023E-01



  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     WATER             1.0000         1.0000         1.0000         1.0000

BLOCK:  RB-302   MODEL: HEATER
------------------------------
  INLET STREAM:           S-409
  INLET HEAT STREAM:      HEAT4
  OUTLET STREAM:          S-317
```

```
 PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT         RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)           2074.34         2074.34         0.00000
     MASS(LB/HR   )           37369.8         37369.8         0.00000
     ENTHALPY(BTU/HR  )     -0.241251E+09   -0.241251E+09     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  ***
 TWO    PHASE  PQ  FLASH
 PRESSURE DROP                        PSI                        10.0000
 DUTY FROM INLET HEAT STREAM(S)       BTU/HR                     -0.289994+08
 MAXIMUM NO. ITERATIONS                                          30
 CONVERGENCE TOLERANCE                                            0.000100000



                        ***  RESULTS  ***
 OUTLET TEMPERATURE    F                                      380.29
 OUTLET PRESSURE       PSIA                                   196.00
 OUTLET VAPOR FRACTION                                       0.42023E-01



 V-L PHASE EQUILIBRIUM :

    COMP              F(I)           X(I)           Y(I)           K(I)
    WATER             1.0000         1.0000         1.0000         1.0000

BLOCK:  T-101    MODEL: COMPR
-----------------------------
 INLET STREAM:           S-218
 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)           16740.9         16740.9         0.00000
     MASS(LB/HR   )           369878.         369878.         0.00000
     ENTHALPY(BTU/HR  )     -0.456152E+09   -0.487978E+09    0.652194E-01

                   ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E           0.293342E+07  LB/HR
  PRODUCT STREAMS CO2E        0.293342E+07  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                                      53.6640
    ISENTROPIC EFFICIENCY                                       0.80000
    MECHANICAL EFFICIENCY                                       1.00000

                         ***  RESULTS  ***

    INDICATED  HORSEPOWER REQUIREMENT  HP                 -12,508.0
    BRAKE      HORSEPOWER REQUIREMENT  HP                 -12,508.0
    NET WORK REQUIRED                  HP                 -12,508.0
    POWER LOSSES                       HP                       0.0
    ISENTROPIC HORSEPOWER REQUIREMENT  HP                 -15,634.9
    CALCULATED OUTLET TEMP  F                                -26.9538
    ISENTROPIC TEMPERATURE  F                                -70.4389
    EFFICIENCY (POLYTR/ISENTR) USED                             0.80000
    OUTLET VAPOR FRACTION                                       0.99084
    HEAD DEVELOPED,       FT-LBF/LB                       -83,695.7
    MECHANICAL EFFICIENCY USED                                  1.00000
    INLET HEAT CAPACITY RATIO                                   1.33025
    INLET VOLUMETRIC FLOW RATE , CUFT/HR                  150,837.
    OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                1,398,420.
    INLET  COMPRESSIBILITY FACTOR                               0.90406
    OUTLET COMPRESSIBILITY FACTOR                               0.96534
    AV. ISENT. VOL. EXPONENT                                    1.21336
    AV. ISENT. TEMP EXPONENT                                    1.24255
    AV. ACTUAL VOL. EXPONENT                                    1.14686
    AV. ACTUAL TEMP EXPONENT                                    1.18167

 BLOCK:  T-102    MODEL: COMPR
 -----------------------------
   INLET STREAM:          S-101
   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)          6283.92         6283.92         0.00000
       MASS(LB/HR   )          189837.         189837.         0.00000
       ENTHALPY(BTU/HR  )   -0.230063E+09   -0.236713E+09    0.280951E-01

                    ***  CO2 EQUIVALENT SUMMARY ***
    FEED STREAMS CO2E            25202.9      LB/HR
    PRODUCT STREAMS CO2E         25202.9      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                                      53.6640
    ISENTROPIC EFFICIENCY                                       0.80000
    MECHANICAL EFFICIENCY                                       1.00000
```

```
                    ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP              -2,613.74
   BRAKE      HORSEPOWER REQUIREMENT  HP              -2,613.74
   NET WORK REQUIRED                  HP              -2,613.74
   POWER LOSSES                       HP                   0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP              -3,267.17
   CALCULATED OUTLET TEMP  F                            -37.4871
   ISENTROPIC TEMPERATURE  F                            -59.9360
   EFFICIENCY (POLYTR/ISENTR) USED                        0.80000
   OUTLET VAPOR FRACTION                                  1.00000
   HEAD DEVELOPED,       FT-LBF/LB                   -34,076.7
   MECHANICAL EFFICIENCY USED                             1.00000
   INLET HEAT CAPACITY RATIO                              1.32990
   INLET VOLUMETRIC FLOW RATE , CUFT/HR              116,830.
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR              500,206.
   INLET  COMPRESSIBILITY FACTOR                          0.84974
   OUTLET COMPRESSIBILITY FACTOR                          0.94285
   AV. ISENT. VOL. EXPONENT                               1.14878
   AV. ISENT. TEMP EXPONENT                               1.23166
   AV. ACTUAL VOL. EXPONENT                               1.09733
   AV. ACTUAL TEMP EXPONENT                               1.18182

BLOCK:  T-103    MODEL: COMPR
-----------------------------
  INLET STREAM:           S-305
  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)          572.227         572.227         0.00000
      MASS(LB/HR   )          20884.5         20884.5         0.00000
      ENTHALPY(BTU/HR  )    -0.937930E+07   -0.962404E+07    0.254296E-01

                ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            69231.5      LB/HR
   PRODUCT STREAMS CO2E         69231.5      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                                 53.6640
   ISENTROPIC EFFICIENCY                                  0.80000
   MECHANICAL EFFICIENCY                                  1.00000

                    ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                -96.1846
   BRAKE      HORSEPOWER REQUIREMENT  HP                -96.1846
   NET WORK REQUIRED                  HP                -96.1846
   POWER LOSSES                       HP                  0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP               -120.231
```

```
   CALCULATED OUTLET TEMP  F                               166.662
   ISENTROPIC TEMPERATURE  F                               165.112
   EFFICIENCY (POLYTR/ISENTR) USED                           0.80000
   OUTLET VAPOR FRACTION                                     0.99432
   HEAD DEVELOPED,        FT-LBF/LB                    -11,398.7
   MECHANICAL EFFICIENCY USED                                1.00000
   INLET HEAT CAPACITY RATIO                                 1.17062
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                 46,729.6
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                 69,613.8
   INLET  COMPRESSIBILITY FACTOR                             0.96763
   OUTLET COMPRESSIBILITY FACTOR                             0.97129
   AV. ISENT. VOL. EXPONENT                                  1.11882
   AV. ISENT. TEMP EXPONENT                                  1.11154
   AV. ACTUAL VOL. EXPONENT                                  1.09411
   AV. ACTUAL TEMP EXPONENT                                  1.10457

BLOCK:  T-401    MODEL: COMPR
-----------------------------
  INLET STREAM:          S-404,
  OUTLET STREAM:         S-406
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          3793.85         3793.85         0.00000
      MASS(LB/HR   )          68347.2         68347.2         0.00000
      ENTHALPY(BTU/HR  )      -0.384325E+09   -0.388197E+09    0.997281E-02

                    ***  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                                   206.000
   ISENTROPIC EFFICIENCY                                     0.80000
   MECHANICAL EFFICIENCY                                     1.00000

                         ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP                -1,521.52
   BRAKE      HORSEPOWER REQUIREMENT  HP                -1,521.52
   NET WORK REQUIRED                  HP                -1,521.52
   POWER LOSSES                       HP                     0.0
   ISENTROPIC HORSEPOWER REQUIREMENT  HP                -1,901.90
   CALCULATED OUTLET TEMP  F                               384.467
   ISENTROPIC TEMPERATURE  F                               384.467
   EFFICIENCY (POLYTR/ISENTR) USED                           0.80000
   OUTLET VAPOR FRACTION                                     0.95971
   HEAD DEVELOPED,        FT-LBF/LB                    -55,097.6
   MECHANICAL EFFICIENCY USED                                1.00000
   INLET HEAT CAPACITY RATIO                                 1.43709
```

```
  INLET VOLUMETRIC FLOW RATE , CUFT/HR                72,687.4
  OUTLET VOLUMETRIC FLOW RATE, CUFT/HR               151,123.
  INLET  COMPRESSIBILITY FACTOR                            0.89696
  OUTLET COMPRESSIBILITY FACTOR                            0.90584
  AV. ISENT. VOL. EXPONENT                                 1.13878
  AV. ISENT. TEMP EXPONENT                                 1.12661
  AV. ACTUAL VOL. EXPONENT                                 1.11146
  AV. ACTUAL TEMP EXPONENT                                 1.12661

BLOCK:  V-101-2  MODEL: MIXER
-----------------------------
 INLET STREAMS:         S-102       S-104       S-103
 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)           23597.0         23597.0         0.00000
     MASS(LB/HR   )           580599.         580599.       -0.200509E-15
     ENTHALPY(BTU/HR  )      -0.734316E+09   -0.734316E+09    0.162341E-15

                    ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E           0.302786E+07  LB/HR
  PRODUCT STREAMS CO2E        0.302786E+07  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:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  V-103    MODEL: MIXER
-----------------------------
 INLET STREAMS:         S-109       S-220
 OUTLET STREAM:         S-220,
 PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)           11566.8         11566.8         0.00000
     MASS(LB/HR   )           290043.         290043.         0.00000
     ENTHALPY(BTU/HR  )      -0.145901E+08   -0.145901E+08   -0.255330E-15

                    ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E             200419.      LB/HR
  PRODUCT STREAMS CO2E          200419.      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:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  V-201    MODEL: VALVE
-----------------------------
  INLET STREAM:           S-205
  OUTLET STREAM:          S-206
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            365.791         365.791         0.00000
      MASS(LB/HR   )            17906.5         17906.5         0.00000
      ENTHALPY(BTU/HR  )      -0.365627E+07   -0.365627E+07     0.00000

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             33131.7      LB/HR
   PRODUCT STREAMS CO2E          33131.7      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  ***

   VALVE OUTLET PRESSURE     PSIA                           11.8000
   VALVE FLOW COEF CALC.                                   NO

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

                         ***  RESULTS  ***

   VALVE PRESSURE DROP       PSI                           718.200

BLOCK:  V-202    MODEL: VALVE
-----------------------------
  INLET STREAM:           S-202
  OUTLET STREAM:          S-207
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            458.147         458.147         0.00000
      MASS(LB/HR   )            29529.9         29529.9         0.00000
      ENTHALPY(BTU/HR  )       0.155143E+07    0.155143E+07     0.00000

                     ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E             19945.6      LB/HR
   PRODUCT STREAMS CO2E          19945.6      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 OUTLET PRESSURE     PSIA                          11.8000
   VALVE FLOW COEF CALC.                                  NO

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

                    ***  RESULTS  ***

   VALVE PRESSURE DROP       PSI                          288.399

BLOCK:  V-203    MODEL: VALVE
-----------------------------
  INLET STREAM:          S-203
  OUTLET STREAM:         S-208
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           512.796         512.796         0.00000
      MASS(LB/HR   )           38836.3         38836.3         0.00000
      ENTHALPY(BTU/HR  )     0.453366E+07    0.453366E+07     0.00000

                ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            9965.80      LB/HR
   PRODUCT STREAMS CO2E         9965.80      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                          11.8000
   VALVE FLOW COEF CALC.                                  NO

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

                    ***  RESULTS  ***

   VALVE PRESSURE DROP       PSI                          114.040

BLOCK:  V-203-5  MODEL: MIXER
-----------------------------
  INLET STREAMS:         S-209       S-208       S-207       S-206
  OUTLET STREAM:         S-210
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

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

```
   TOTAL BALANCE
      MOLE(LBMOL/HR)            2060.30         2060.31       -0.247041E-05
      MASS(LB/HR   )            149159.         149159.       -0.299691E-05
      ENTHALPY(BTU/HR  )       0.597930E+07    0.597939E+07   -0.151762E-04

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E              69232.1      LB/HR
   PRODUCT STREAMS CO2E           69231.5      LB/HR
   NET STREAMS CO2E PRODUCTION -0.574376      LB/HR
   UTILITIES CO2E PRODUCTION      0.00000      LB/HR
   TOTAL CO2E PRODUCTION         -0.574376      LB/HR

                       ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                         30
  CONVERGENCE TOLERANCE                                           0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  V-206    MODEL: FSPLIT
------------------------------
  INLET STREAM:            S-219
  OUTLET STREAMS:          S-221       S-220
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            10748.3         10748.3         0.00000
      MASS(LB/HR   )            61564.4         61564.4         0.00000
      ENTHALPY(BTU/HR  )      -0.828870E+08   -0.828870E+08     0.00000

                   ***  CO2 EQUIVALENT SUMMARY ***
   FEED STREAMS CO2E            0.114078E+07  LB/HR
   PRODUCT STREAMS CO2E         0.114078E+07  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  ***

 FRACTION OF FLOW                 STRM=S-221    FRAC=         0.82431

                        ***  RESULTS  ***

 STREAM= S-221           SPLIT=          0.82431     KEY=  0    STREAM-ORDER=
1
        S-220                                       0.17569                 0
2

BLOCK:  V-401-3  MODEL: MIXER
-----------------------------
  INLET STREAMS:          S-402       S-317       S-217       S-308
  OUTLET STREAM:          S-403
  PROPERTY OPTION SET:   NRTL-RK   RENON (NRTL) / REDLICH-KWONG

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

```
  TOTAL BALANCE
     MOLE(LBMOL/HR)            61691.1         61691.1         0.00000
     MASS(LB/HR   )          0.111138E+07    0.111138E+07   -0.209497E-15
     ENTHALPY(BTU/HR  )      -0.755446E+10   -0.755446E+10    0.252480E-15

                  ***  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      FLASH
 MAXIMUM NO. ITERATIONS                                        30
 CONVERGENCE TOLERANCE                                          0.000100000
 OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  V-404    MODEL: MIXER
-----------------------------
 INLET STREAMS:          S-221       S-410
 OUTLET STREAM:          S-221,
 PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                IN               OUT        RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)            54270.9         54270.9         0.00000
     MASS(LB/HR   )          0.136087E+07    0.136087E+07     0.00000
     ENTHALPY(BTU/HR  )      -0.684562E+08   -0.684562E+08   -0.217674E-15

                  ***  CO2 EQUIVALENT SUMMARY ***
  FEED STREAMS CO2E             940357.      LB/HR
  PRODUCT STREAMS CO2E          940357.      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:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  V-405    MODEL: FSPLIT
------------------------------
 INLET STREAM:           S-404
 OUTLET STREAMS:         S-405       S-404,
 PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                  ***  MASS AND ENERGY BALANCE  ***
                                IN               OUT        RELATIVE DIFF.
  TOTAL BALANCE
     MOLE(LBMOL/HR)            61691.1         61691.1         0.00000
     MASS(LB/HR   )          0.111138E+07    0.111138E+07   -0.209497E-15
     ENTHALPY(BTU/HR  )      -0.624944E+10   -0.624944E+10    0.152601E-15
```

```
                    ***  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  ***

 FRACTION OF FLOW                  STRM=S-404,   FRAC=         0.061498

                         ***  RESULTS  ***

 STREAM= S-405          SPLIT=          0.93850     KEY=  0    STREAM-ORDER=
2
        S-404,                                    0.061498                0
1

BLOCK:  V-406-7  MODEL: FSPLIT
------------------------------
  INLET STREAM:           S-406
  OUTLET STREAMS:         S-408       S-409       S-407
  PROPERTY OPTION SET:    NRTL-RK   RENON (NRTL) / REDLICH-KWONG

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           3793.85         3793.85        0.119864E-15
      MASS(LB/HR   )           68347.2         68347.2         0.00000
      ENTHALPY(BTU/HR  )     -0.388197E+09   -0.388197E+09     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  ***

 FRACTION OF FLOW                  STRM=S-408    FRAC=         0.17030
                                   STRM=S-409    FRAC=         0.54676

                         ***  RESULTS  ***

 STREAM= S-408          SPLIT=          0.17030     KEY=  0    STREAM-ORDER=
1
        S-409                                     0.54676                 0
2
        S-407                                     0.28294                 0
3
```

A-5.4.1. TPFQ Profile for COL-301

| Stage | Temperature | Pressure | Heat duty | Liquid from (Mass) | Vapor from (Mass) | Liquid enthalpy | Vapor enthalpy | Liquid flow (Mass) | Vapor flow (Mass) |
|---|---|---|---|---|---|---|---|---|---|
| | F | psia | Btu/hr | lb/hr | lb/hr | Btu/lbmol | Btu/lbmol | lb/hr | lb/hr |
| 1 | 186 | 83.0 | -548155 | 2104 | 20449 | 17461 | -16513 | 2104 | 20449 |
| 2 | 209 | 93.0 | 0 | 2179 | 22553 | 18086 | -13986 | 2179 | 22553 |
| 3 | 211 | 93.2 | 0 | 2163 | 22628 | 17872 | -13918 | 2163 | 22628 |
| 4 | 211 | 93.3 | 0 | 2150 | 22612 | 17719 | -13945 | 2150 | 22612 |
| 5 | 212 | 93.5 | 0 | 2140 | 22599 | 17619 | -13964 | 2140 | 22599 |
| 6 | 212 | 93.6 | 0 | 2131 | 22589 | 17545 | -13978 | 2131 | 22589 |
| 7 | 212 | 93.8 | 0 | 2123 | 22580 | 17487 | -13989 | 2123 | 22580 |
| 8 | 212 | 93.9 | 0 | 2115 | 22572 | 17438 | -13999 | 2115 | 22572 |
| 9 | 212 | 94.1 | 0 | 2108 | 22564 | 17395 | -14007 | 2108 | 22564 |
| 10 | 212 | 94.2 | 0 | 2102 | 22558 | 17358 | -14014 | 2102 | 22558 |
| 11 | 213 | 94.4 | 0 | 2095 | 22551 | 17322 | -14021 | 2095 | 22551 |
| 12 | 213 | 94.5 | 0 | 2089 | 22544 | 17288 | -14028 | 2089 | 22544 |
| 13 | 213 | 94.7 | 0 | 2082 | 22538 | 17252 | -14034 | 2082 | 22538 |
| 14 | 213 | 94.8 | 0 | 2075 | 22531 | 17213 | -14041 | 2075 | 22531 |
| 15 | 213 | 95.0 | 0 | 2067 | 22524 | 17166 | -14048 | 2067 | 22524 |
| 16 | 213 | 95.1 | 0 | 2057 | 22516 | 17108 | -14057 | 2057 | 22516 |
| 17 | 213 | 95.3 | 0 | 2047 | 22507 | 17033 | -14067 | 2047 | 22507 |
| 18 | 214 | 95.4 | 0 | 2038 | 22496 | 16935 | -14078 | 2038 | 22496 |
| 19 | 214 | 95.6 | 0 | 2053 | 22487 | 16807 | -14091 | 2053 | 22487 |
| 20 | 214 | 95.7 | 0 | 2296 | 22502 | 16661 | -14088 | 2296 | 22502 |
| 21 | 210 | 95.9 | 0 | 4541 | 22745 | 16592 | -13934 | 4541 | 22745 |
| 22 | 190 | 96.0 | 0 | 174113 | 21844 | 12445 | -7877 | 174113 | 21844 |
| 23 | 283 | 96.2 | 0 | 221917 | 48283 | 20266 | 17208 | 221917 | 48283 |
| 24 | 317 | 96.3 | 0 | 247393 | 96087 | 23942 | 31976 | 247393 | 96087 |
| 25 | 326 | 96.5 | 0 | 255826 | 121562 | 25200 | 37085 | 255826 | 121562 |
| 26 | 329 | 96.6 | 0 | 258622 | 129996 | 25624 | 38784 | 258622 | 129996 |
| 27 | 330 | 96.8 | 0 | 259600 | 132791 | 25771 | 39353 | 259600 | 132791 |

| Stage | Temperature | Pressure | Heat duty | Liquid from (Mass) | Vapor from (Mass) | Liquid enthalpy | Vapor enthalpy | Liquid flow (Mass) | Vapor flow (Mass) |
|---|---|---|---|---|---|---|---|---|---|
| 28 | 331 | 96.9 | 0 | 259992 | 133769 | 25827 | 39549 | 259992 | 133769 |
| 29 | 331 | 97.1 | 0 | 260195 | 134162 | 25852 | 39621 | 260195 | 134162 |
| 30 | 331 | 97.2 | 0 | 260335 | 134365 | 25867 | 39649 | 260335 | 134365 |
| 31 | 331 | 97.4 | 0 | 260454 | 134505 | 25877 | 39662 | 260454 | 134505 |
| 32 | 332 | 97.5 | 0 | 260565 | 134623 | 25886 | 39669 | 260565 | 134623 |
| 33 | 332 | 97.7 | 0 | 260673 | 134734 | 25894 | 39675 | 260673 | 134734 |
| 34 | 332 | 97.8 | 0 | 260780 | 134843 | 25902 | 39679 | 260780 | 134843 |
| 35 | 332 | 98.0 | 0 | 260887 | 134950 | 25910 | 39683 | 260887 | 134950 |
| 36 | 332 | 98.1 | 0 | 260993 | 135056 | 25918 | 39687 | 260993 | 135056 |
| 37 | 332 | 98.3 | 0 | 261100 | 135163 | 25925 | 39691 | 261100 | 135163 |
| 38 | 333 | 98.4 | 0 | 261206 | 135269 | 25933 | 39694 | 261206 | 135269 |
| 39 | 333 | 98.6 | 0 | 261312 | 135375 | 25941 | 39698 | 261312 | 135375 |
| 40 | 333 | 98.7 | 0 | 261418 | 135481 | 25949 | 39702 | 261418 | 135481 |
| 41 | 333 | 98.9 | 0 | 261524 | 135587 | 25957 | 39706 | 261524 | 135587 |
| 42 | 333 | 99.0 | 0 | 261630 | 135693 | 25964 | 39709 | 261630 | 135693 |
| 43 | 333 | 99.2 | 0 | 261736 | 135799 | 25972 | 39713 | 261736 | 135799 |
| 44 | 333 | 99.3 | 0 | 261842 | 135905 | 25980 | 39717 | 261842 | 135905 |
| 45 | 334 | 99.5 | 0 | 261948 | 136011 | 25988 | 39721 | 261948 | 136011 |
| 46 | 334 | 99.6 | 0 | 262054 | 136117 | 25995 | 39724 | 262054 | 136117 |
| 47 | 334 | 99.8 | 0 | 262159 | 136223 | 26003 | 39728 | 262159 | 136223 |
| 48 | 334 | 99.9 | 0 | 262265 | 136329 | 26011 | 39732 | 262265 | 136329 |
| 49 | 334 | 100.1 | 0 | 262371 | 136435 | 26018 | 39735 | 262371 | 136435 |
| 50 | 334 | 100.2 | 0 | 262477 | 136541 | 26026 | 39739 | 262477 | 136541 |
| 51 | 334 | 100.4 | 0 | 262584 | 136647 | 26033 | 39742 | 262584 | 136647 |
| 52 | 335 | 100.5 | 0 | 262691 | 136753 | 26041 | 39746 | 262691 | 136753 |
| 53 | 335 | 100.7 | 0 | 262799 | 136860 | 26048 | 39749 | 262799 | 136860 |
| 54 | 335 | 100.8 | 0 | 262909 | 136969 | 26055 | 39751 | 262909 | 136969 |
| 55 | 335 | 101.0 | 0 | 263022 | 137079 | 26060 | 39753 | 263022 | 137079 |
| 56 | 335 | 101.1 | 0 | 263141 | 137192 | 26065 | 39753 | 263141 | 137192 |

| Stage | Temperature | Pressure | Heat duty | Liquid from (Mass) | Vapor from (Mass) | Liquid enthalpy | Vapor enthalpy | Liquid flow (Mass) | Vapor flow (Mass) |
|---|---|---|---|---|---|---|---|---|---|
| 57 | 335 | 101.3 | 0 | 263269 | 137310 | 26067 | 39751 | 263269 | 137310 |
| 58 | 335 | 101.4 | 0 | 263413 | 137438 | 26065 | 39745 | 263413 | 137438 |
| 59 | 336 | 101.6 | 0 | 263586 | 137583 | 26056 | 39731 | 263586 | 137583 |
| 60 | 336 | 101.7 | 0 | 263806 | 137755 | 26034 | 39704 | 263806 | 137755 |
| 61 | 336 | 101.9 | 0 | 264108 | 137975 | 25987 | 39653 | 264108 | 137975 |
| 62 | 337 | 102.0 | 0 | 264551 | 138278 | 25897 | 39559 | 264551 | 138278 |
| 63 | 338 | 102.2 | 0 | 265214 | 138720 | 25724 | 39386 | 265214 | 138720 |
| 64 | 340 | 102.3 | 0 | 264044 | 139384 | 25387 | 39071 | 264044 | 139384 |
| 65 | 349 | 102.5 | 19604403 | 125831 | 138214 | 23436 | 38680 | 125831 | 138214 |

A-5.4.2. Liquid Mass Composition Profile for COL-301

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E+00 | 2.21E-16 | 2.56E-03 | 2.41E-02 | 1.72E-03 | 4.32E-03 | 5.07E-04 | 7.91E-01 | 1.67E-01 | 9.08E-03 | 1.51E-05 |
| 2.00E+00 | 3.05E-16 | 2.11E-03 | 2.30E-02 | 1.66E-03 | 4.16E-03 | 5.12E-04 | 7.55E-01 | 1.98E-01 | 1.48E-02 | 3.30E-05 |
| 3.00E+00 | 3.09E-16 | 2.07E-03 | 2.28E-02 | 1.65E-03 | 4.13E-03 | 5.13E-04 | 7.37E-01 | 2.12E-01 | 2.01E-02 | 5.93E-05 |
| 4.00E+00 | 3.11E-16 | 2.06E-03 | 2.28E-02 | 1.65E-03 | 4.12E-03 | 5.15E-04 | 7.27E-01 | 2.17E-01 | 2.47E-02 | 9.69E-05 |
| 5.00E+00 | 3.12E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.12E-03 | 5.16E-04 | 7.22E-01 | 2.18E-01 | 2.88E-02 | 1.50E-04 |
| 6.00E+00 | 3.13E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.12E-03 | 5.17E-04 | 7.19E-01 | 2.17E-01 | 3.22E-02 | 2.26E-04 |
| 7.00E+00 | 3.14E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.13E-03 | 5.18E-04 | 7.17E-01 | 2.17E-01 | 3.52E-02 | 3.33E-04 |
| 8.00E+00 | 3.15E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.13E-03 | 5.19E-04 | 7.15E-01 | 2.16E-01 | 3.77E-02 | 4.83E-04 |
| 9.00E+00 | 3.16E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.13E-03 | 5.20E-04 | 7.13E-01 | 2.15E-01 | 3.97E-02 | 6.95E-04 |
| 1.00E+01 | 3.17E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.14E-03 | 5.21E-04 | 7.12E-01 | 2.14E-01 | 4.14E-02 | 9.91E-04 |
| 1.10E+01 | 3.18E-16 | 2.05E-03 | 2.28E-02 | 1.65E-03 | 4.14E-03 | 5.21E-04 | 7.11E-01 | 2.14E-01 | 4.28E-02 | 1.41E-03 |
| 1.20E+01 | 3.19E-16 | 2.05E-03 | 2.29E-02 | 1.65E-03 | 4.14E-03 | 5.22E-04 | 7.10E-01 | 2.13E-01 | 4.39E-02 | 1.98E-03 |
| 1.30E+01 | 3.20E-16 | 2.05E-03 | 2.29E-02 | 1.66E-03 | 4.15E-03 | 5.23E-04 | 7.09E-01 | 2.12E-01 | 4.48E-02 | 2.79E-03 |
| 1.40E+01 | 3.21E-16 | 2.05E-03 | 2.29E-02 | 1.66E-03 | 4.15E-03 | 5.23E-04 | 7.08E-01 | 2.11E-01 | 4.54E-02 | 3.91E-03 |
| 1.50E+01 | 3.22E-16 | 2.05E-03 | 2.29E-02 | 1.66E-03 | 4.15E-03 | 5.24E-04 | 7.07E-01 | 2.11E-01 | 4.57E-02 | 5.45E-03 |
| 1.60E+01 | 3.23E-16 | 2.05E-03 | 2.29E-02 | 1.66E-03 | 4.15E-03 | 5.24E-04 | 7.05E-01 | 2.10E-01 | 4.59E-02 | 7.58E-03 |

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.70E+01 | 3.24E-16 | 2.04E-03 | 2.29E-02 | 1.66E-03 | 4.16E-03 | 5.25E-04 | 7.03E-01 | 2.09E-01 | 4.59E-02 | 1.05E-02 |
| 1.80E+01 | 3.25E-16 | 2.04E-03 | 2.29E-02 | 1.66E-03 | 4.16E-03 | 5.25E-04 | 7.01E-01 | 2.08E-01 | 4.56E-02 | 1.45E-02 |
| 1.90E+01 | 3.26E-16 | 2.04E-03 | 2.29E-02 | 1.66E-03 | 4.16E-03 | 5.26E-04 | 6.98E-01 | 2.06E-01 | 4.50E-02 | 1.97E-02 |
| 2.00E+01 | 3.26E-16 | 2.05E-03 | 2.30E-02 | 1.67E-03 | 4.17E-03 | 5.27E-04 | 6.96E-01 | 2.03E-01 | 4.34E-02 | 2.58E-02 |
| 2.10E+01 | 3.19E-16 | 2.18E-03 | 2.38E-02 | 1.72E-03 | 4.28E-03 | 5.40E-04 | 7.08E-01 | 1.95E-01 | 3.74E-02 | 2.65E-02 |
| 2.20E+01 | 1.77E-22 | 2.69E-03 | 2.87E-02 | 2.01E-03 | 5.15E-03 | 7.00E-04 | 6.07E-01 | 2.29E-01 | 5.61E-02 | 6.97E-02 |
| 2.30E+01 | 1.63E-28 | 2.26E-04 | 1.39E-02 | 8.72E-04 | 3.83E-03 | 3.63E-04 | 6.71E-01 | 2.06E-01 | 4.73E-02 | 5.70E-02 |
| 2.40E+01 | 1.54E-34 | 1.09E-05 | 4.74E-03 | 2.72E-04 | 1.96E-03 | 1.28E-04 | 6.99E-01 | 1.98E-01 | 4.41E-02 | 5.23E-02 |
| 2.50E+01 | 1.47E-40 | 4.52E-07 | 1.47E-03 | 7.75E-05 | 9.05E-04 | 4.03E-05 | 7.08E-01 | 1.95E-01 | 4.32E-02 | 5.09E-02 |
| 2.60E+01 | 1.41E-46 | 1.80E-08 | 4.48E-04 | 2.16E-05 | 4.06E-04 | 1.24E-05 | 7.11E-01 | 1.95E-01 | 4.29E-02 | 5.05E-02 |
| 2.70E+01 | 1.36E-52 | 7.06E-10 | 1.35E-04 | 6.00E-06 | 1.81E-04 | 3.77E-06 | 7.12E-01 | 1.94E-01 | 4.28E-02 | 5.04E-02 |
| 2.80E+01 | 1.31E-58 | 2.76E-11 | 4.08E-05 | 1.66E-06 | 8.06E-05 | 1.15E-06 | 7.12E-01 | 1.94E-01 | 4.28E-02 | 5.03E-02 |
| 2.90E+01 | 1.27E-64 | 1.08E-12 | 1.23E-05 | 4.61E-07 | 3.59E-05 | 3.49E-07 | 7.13E-01 | 1.94E-01 | 4.28E-02 | 5.03E-02 |
| 3.00E+01 | 1.24E-70 | 4.22E-14 | 3.72E-06 | 1.28E-07 | 1.60E-05 | 1.06E-07 | 7.13E-01 | 1.94E-01 | 4.28E-02 | 5.03E-02 |
| 3.10E+01 | 1.21E-76 | 1.65E-15 | 1.12E-06 | 3.56E-08 | 7.10E-06 | 3.23E-08 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.03E-02 |
| 3.20E+01 | 1.18E-82 | 6.45E-17 | 3.39E-07 | 9.89E-09 | 3.16E-06 | 9.84E-09 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.30E+01 | 1.16E-88 | 2.52E-18 | 1.03E-07 | 2.75E-09 | 1.41E-06 | 3.00E-09 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.40E+01 | 1.14E-94 | 9.87E-20 | 3.11E-08 | 7.67E-10 | 6.29E-07 | 9.15E-10 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.50E+01 | 1.12E-100 | 3.86E-21 | 9.41E-09 | 2.14E-10 | 2.81E-07 | 2.79E-10 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.60E+01 | 1.11E-106 | 9.95E-23 | 2.85E-09 | 5.97E-11 | 1.25E-07 | 8.52E-11 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.70E+01 | 1.10E-112 | 2.56E-24 | 8.66E-10 | 1.67E-11 | 5.59E-08 | 2.60E-11 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.80E+01 | 1.09E-118 | 6.61E-26 | 2.63E-10 | 4.66E-12 | 2.50E-08 | 7.96E-12 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.02E-02 |
| 3.90E+01 | 1.09E-124 | 1.71E-27 | 8.00E-11 | 1.30E-12 | 1.12E-08 | 2.44E-12 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.01E-02 |
| 4.00E+01 | 1.09E-130 | 4.40E-29 | 2.43E-11 | 3.65E-13 | 5.00E-09 | 7.46E-13 | 7.13E-01 | 1.94E-01 | 4.27E-02 | 5.01E-02 |
| 4.10E+01 | 1.09E-136 | 1.14E-30 | 7.41E-12 | 1.02E-13 | 2.24E-09 | 2.29E-13 | 7.13E-01 | 1.94E-01 | 4.26E-02 | 5.01E-02 |
| 4.20E+01 | 1.09E-142 | 2.93E-32 | 2.26E-12 | 2.87E-14 | 1.00E-09 | 7.01E-14 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.01E-02 |
| 4.30E+01 | 1.10E-148 | 7.56E-34 | 6.89E-13 | 8.07E-15 | 4.49E-10 | 2.15E-14 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.01E-02 |
| 4.40E+01 | 1.11E-154 | 1.95E-35 | 2.10E-13 | 2.27E-15 | 2.02E-10 | 6.60E-15 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.01E-02 |
| 4.50E+01 | 1.12E-160 | 5.04E-37 | 6.42E-14 | 6.38E-16 | 9.04E-11 | 2.03E-15 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.01E-02 |
| 4.60E+01 | 1.13E-166 | 1.30E-38 | 1.96E-14 | 1.80E-16 | 4.06E-11 | 6.23E-16 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.00E-02 |

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 4.70E+01 | 1.15E-172 | 3.36E-40 | 6.01E-15 | 5.07E-17 | 1.82E-11 | 1.92E-16 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.00E-02 |
| 4.80E+01 | 1.17E-178 | 8.68E-42 | 1.84E-15 | 1.43E-17 | 8.19E-12 | 5.89E-17 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.00E-02 |
| 4.90E+01 | 1.20E-184 | 2.24E-43 | 5.64E-16 | 4.04E-18 | 3.68E-12 | 1.82E-17 | 7.14E-01 | 1.94E-01 | 4.26E-02 | 5.00E-02 |
| 5.00E+01 | 1.22E-190 | 5.79E-45 | 1.73E-16 | 1.14E-18 | 1.66E-12 | 5.59E-18 | 7.14E-01 | 1.93E-01 | 4.26E-02 | 5.00E-02 |
| 5.10E+01 | 1.26E-196 | 1.50E-46 | 5.31E-17 | 3.23E-19 | 7.46E-13 | 1.72E-18 | 7.14E-01 | 1.93E-01 | 4.26E-02 | 5.00E-02 |
| 5.20E+01 | 1.29E-202 | 3.87E-48 | 1.63E-17 | 9.15E-20 | 3.36E-13 | 5.32E-19 | 7.14E-01 | 1.93E-01 | 4.25E-02 | 5.00E-02 |
| 5.30E+01 | 1.33E-208 | 1.00E-49 | 5.01E-18 | 2.59E-20 | 1.51E-13 | 1.64E-19 | 7.14E-01 | 1.93E-01 | 4.25E-02 | 4.99E-02 |
| 5.40E+01 | 1.38E-214 | 2.58E-51 | 1.54E-18 | 7.35E-21 | 6.82E-14 | 5.08E-20 | 7.14E-01 | 1.94E-01 | 4.25E-02 | 4.99E-02 |
| 5.50E+01 | 1.43E-220 | 6.68E-53 | 4.75E-19 | 1.51E-21 | 3.08E-14 | 1.57E-20 | 7.14E-01 | 1.94E-01 | 4.25E-02 | 4.99E-02 |
| 5.60E+01 | 1.48E-226 | 1.73E-54 | 1.46E-19 | 3.09E-22 | 1.39E-14 | 4.85E-21 | 7.14E-01 | 1.94E-01 | 4.25E-02 | 4.99E-02 |
| 5.70E+01 | 1.54E-232 | 4.47E-56 | 4.51E-20 | 6.35E-23 | 6.27E-15 | 1.10E-21 | 7.13E-01 | 1.94E-01 | 4.26E-02 | 4.99E-02 |
| 5.80E+01 | 1.61E-238 | 1.15E-57 | 1.39E-20 | 1.30E-23 | 2.83E-15 | 2.47E-22 | 7.12E-01 | 1.95E-01 | 4.26E-02 | 4.99E-02 |
| 5.90E+01 | 1.69E-244 | 2.98E-59 | 4.30E-21 | 2.68E-24 | 1.28E-15 | 5.59E-23 | 7.11E-01 | 1.96E-01 | 4.27E-02 | 5.00E-02 |
| 6.00E+01 | 1.78E-250 | 7.69E-61 | 9.68E-22 | 5.52E-25 | 5.76E-16 | 1.27E-23 | 7.09E-01 | 1.98E-01 | 4.29E-02 | 5.01E-02 |
| 6.10E+01 | 1.88E-256 | 1.98E-62 | 2.18E-22 | 1.14E-25 | 2.59E-16 | 2.87E-24 | 7.04E-01 | 2.02E-01 | 4.34E-02 | 5.04E-02 |
| 6.20E+01 | 2.00E-262 | 5.07E-64 | 4.89E-23 | 2.33E-26 | 1.16E-16 | 6.50E-25 | 6.97E-01 | 2.08E-01 | 4.43E-02 | 5.11E-02 |
| 6.30E+01 | 2.14E-268 | 1.29E-65 | 1.09E-23 | 4.78E-27 | 5.12E-17 | 1.47E-25 | 6.84E-01 | 2.18E-01 | 4.62E-02 | 5.26E-02 |
| 6.40E+01 | 2.33E-274 | 3.23E-67 | 2.39E-24 | 9.62E-28 | 2.20E-17 | 3.29E-26 | 6.60E-01 | 2.33E-01 | 5.02E-02 | 5.64E-02 |
| 6.50E+01 | 2.67E-280 | 7.40E-69 | 4.71E-25 | 1.76E-28 | 6.28E-18 | 6.83E-27 | 5.58E-01 | 2.76E-01 | 7.27E-02 | 9.33E-02 |

A-5.4.3. Vapor Mass Composition Profile for COL-301

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.00E+00 | 5.04E-09 | 1.33E-01 | 3.44E-01 | 2.97E-02 | 3.48E-02 | 7.00E-03 | 4.09E-01 | 4.08E-02 | 1.16E-03 | 1.27E-06 |
| 2.00E+00 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.45E-01 | 5.26E-02 | 1.90E-03 | 2.56E-06 |
| 3.00E+00 | 4.55E-09 | 1.20E-01 | 3.13E-01 | 2.70E-02 | 3.18E-02 | 6.37E-03 | 4.43E-01 | 5.60E-02 | 2.48E-03 | 4.32E-06 |
| 4.00E+00 | 4.56E-09 | 1.20E-01 | 3.13E-01 | 2.71E-02 | 3.18E-02 | 6.38E-03 | 4.41E-01 | 5.72E-02 | 2.97E-03 | 6.82E-06 |
| 5.00E+00 | 4.56E-09 | 1.20E-01 | 3.14E-01 | 2.71E-02 | 3.18E-02 | 6.38E-03 | 4.40E-01 | 5.76E-02 | 3.41E-03 | 1.04E-05 |
| 6.00E+00 | 4.56E-09 | 1.20E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.38E-03 | 4.39E-01 | 5.76E-02 | 3.78E-03 | 1.54E-05 |
| 7.00E+00 | 4.56E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.38E-03 | 4.39E-01 | 5.75E-02 | 4.09E-03 | 2.25E-05 |

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 8.00E+00 | 4.56E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.38E-01 | 5.74E-02 | 4.36E-03 | 3.25E-05 |
| 9.00E+00 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.38E-01 | 5.72E-02 | 4.58E-03 | 4.65E-05 |
| 1.00E+01 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.38E-01 | 5.71E-02 | 4.77E-03 | 6.61E-05 |
| 1.10E+01 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.38E-01 | 5.70E-02 | 4.92E-03 | 9.36E-05 |
| 1.20E+01 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.39E-03 | 4.37E-01 | 5.69E-02 | 5.03E-03 | 1.32E-04 |
| 1.30E+01 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.40E-03 | 4.37E-01 | 5.68E-02 | 5.12E-03 | 1.85E-04 |
| 1.40E+01 | 4.57E-09 | 1.21E-01 | 3.14E-01 | 2.71E-02 | 3.19E-02 | 6.40E-03 | 4.37E-01 | 5.67E-02 | 5.19E-03 | 2.59E-04 |
| 1.50E+01 | 4.57E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.19E-02 | 6.40E-03 | 4.37E-01 | 5.66E-02 | 5.23E-03 | 3.61E-04 |
| 1.60E+01 | 4.58E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.19E-02 | 6.40E-03 | 4.37E-01 | 5.64E-02 | 5.25E-03 | 5.01E-04 |
| 1.70E+01 | 4.58E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.20E-02 | 6.40E-03 | 4.37E-01 | 5.63E-02 | 5.25E-03 | 6.94E-04 |
| 1.80E+01 | 4.58E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.20E-02 | 6.41E-03 | 4.36E-01 | 5.61E-02 | 5.23E-03 | 9.56E-04 |
| 1.90E+01 | 4.58E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.20E-02 | 6.41E-03 | 4.36E-01 | 5.60E-02 | 5.19E-03 | 1.31E-03 |
| 2.00E+01 | 4.58E-09 | 1.21E-01 | 3.15E-01 | 2.72E-02 | 3.20E-02 | 6.41E-03 | 4.36E-01 | 5.59E-02 | 5.16E-03 | 1.80E-03 |
| 2.10E+01 | 4.53E-09 | 1.20E-01 | 3.12E-01 | 2.69E-02 | 3.17E-02 | 6.34E-03 | 4.38E-01 | 5.72E-02 | 5.42E-03 | 2.60E-03 |
| 2.20E+01 | 1.83E-15 | 7.51E-02 | 2.55E-01 | 2.08E-02 | 3.02E-02 | 5.66E-03 | 5.22E-01 | 7.75E-02 | 8.76E-03 | 5.47E-03 |
| 2.30E+01 | 6.37E-22 | 9.72E-03 | 1.03E-01 | 7.26E-03 | 1.86E-02 | 2.53E-03 | 7.32E-01 | 1.06E-01 | 1.26E-02 | 8.26E-03 |
| 2.40E+01 | 3.77E-28 | 5.21E-04 | 3.20E-02 | 2.01E-03 | 8.85E-03 | 8.38E-04 | 8.17E-01 | 1.15E-01 | 1.41E-02 | 9.47E-03 |
| 2.50E+01 | 3.14E-34 | 2.22E-05 | 9.65E-03 | 5.53E-04 | 3.99E-03 | 2.60E-04 | 8.44E-01 | 1.17E-01 | 1.45E-02 | 9.83E-03 |
| 2.60E+01 | 2.89E-40 | 8.89E-07 | 2.90E-03 | 1.52E-04 | 1.78E-03 | 7.93E-05 | 8.53E-01 | 1.18E-01 | 1.46E-02 | 9.95E-03 |
| 2.70E+01 | 2.74E-46 | 3.50E-08 | 8.73E-04 | 4.21E-05 | 7.91E-04 | 2.41E-05 | 8.56E-01 | 1.18E-01 | 1.47E-02 | 9.99E-03 |
| 2.80E+01 | 2.63E-52 | 1.37E-09 | 2.63E-04 | 1.16E-05 | 3.52E-04 | 7.32E-06 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 2.90E+01 | 2.55E-58 | 5.36E-11 | 7.91E-05 | 3.22E-06 | 1.56E-04 | 2.22E-06 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.00E+01 | 2.47E-64 | 2.09E-12 | 2.38E-05 | 8.94E-07 | 6.94E-05 | 6.76E-07 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.10E+01 | 2.40E-70 | 8.18E-14 | 7.19E-06 | 2.48E-07 | 3.09E-05 | 2.05E-07 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.20E+01 | 2.34E-76 | 3.19E-15 | 2.17E-06 | 6.88E-08 | 1.37E-05 | 6.25E-08 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.30E+01 | 2.29E-82 | 1.25E-16 | 6.56E-07 | 1.91E-08 | 6.12E-06 | 1.90E-08 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.40E+01 | 2.24E-88 | 4.88E-18 | 1.98E-07 | 5.32E-09 | 2.73E-06 | 5.80E-09 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.50E+01 | 2.21E-94 | 1.91E-19 | 6.00E-08 | 1.48E-09 | 1.22E-06 | 1.77E-09 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.60E+01 | 2.17E-100 | 7.45E-21 | 1.82E-08 | 4.13E-10 | 5.42E-07 | 5.39E-10 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.00E-02 |
| 3.70E+01 | 2.15E-106 | 1.92E-22 | 5.51E-09 | 1.15E-10 | 2.42E-07 | 1.65E-10 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.01E-02 |

| Stage | Hydrogen | Methane | Ethane | Ethylene | Propane | Propylene | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|---|---|---|---|---|---|
| 3.80E+01 | 2.13E-112 | 4.95E-24 | 1.67E-09 | 3.22E-11 | 1.08E-07 | 5.03E-11 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.01E-02 |
| 3.90E+01 | 2.11E-118 | 1.28E-25 | 5.08E-10 | 8.99E-12 | 4.82E-08 | 1.54E-11 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.01E-02 |
| 4.00E+01 | 2.10E-124 | 3.29E-27 | 1.54E-10 | 2.51E-12 | 2.16E-08 | 4.70E-12 | 8.57E-01 | 1.18E-01 | 1.47E-02 | 1.01E-02 |
| 4.10E+01 | 2.10E-130 | 8.48E-29 | 4.69E-11 | 7.04E-13 | 9.64E-09 | 1.44E-12 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.20E+01 | 2.10E-136 | 2.19E-30 | 1.43E-11 | 1.97E-13 | 4.31E-09 | 4.40E-13 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.30E+01 | 2.10E-142 | 5.64E-32 | 4.35E-12 | 5.53E-14 | 1.93E-09 | 1.35E-13 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.40E+01 | 2.11E-148 | 1.46E-33 | 1.33E-12 | 1.55E-14 | 8.65E-10 | 4.14E-14 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.50E+01 | 2.13E-154 | 3.76E-35 | 4.05E-13 | 4.37E-15 | 3.88E-10 | 1.27E-14 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.60E+01 | 2.15E-160 | 9.69E-37 | 1.24E-13 | 1.23E-15 | 1.74E-10 | 3.90E-15 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.70E+01 | 2.18E-166 | 2.50E-38 | 3.78E-14 | 3.46E-16 | 7.81E-11 | 1.20E-15 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.80E+01 | 2.21E-172 | 6.46E-40 | 1.16E-14 | 9.74E-17 | 3.51E-11 | 3.68E-16 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 4.90E+01 | 2.25E-178 | 1.67E-41 | 3.54E-15 | 2.75E-17 | 1.57E-11 | 1.13E-16 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.00E+01 | 2.30E-184 | 4.31E-43 | 1.08E-15 | 7.76E-18 | 7.08E-12 | 3.49E-17 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.10E+01 | 2.35E-190 | 1.11E-44 | 3.32E-16 | 2.19E-18 | 3.18E-12 | 1.07E-17 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.20E+01 | 2.41E-196 | 2.87E-46 | 1.02E-16 | 6.20E-19 | 1.43E-12 | 3.31E-18 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.30E+01 | 2.48E-202 | 7.42E-48 | 3.13E-17 | 1.76E-19 | 6.45E-13 | 1.02E-18 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.40E+01 | 2.56E-208 | 1.92E-49 | 9.62E-18 | 4.97E-20 | 2.90E-13 | 3.15E-19 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.50E+01 | 2.64E-214 | 4.96E-51 | 2.96E-18 | 1.41E-20 | 1.31E-13 | 9.73E-20 | 8.57E-01 | 1.18E-01 | 1.48E-02 | 1.01E-02 |
| 5.60E+01 | 2.74E-220 | 1.28E-52 | 9.11E-19 | 2.89E-21 | 5.90E-14 | 3.01E-20 | 8.56E-01 | 1.19E-01 | 1.48E-02 | 1.02E-02 |
| 5.70E+01 | 2.84E-226 | 3.31E-54 | 2.81E-19 | 5.92E-22 | 2.66E-14 | 9.30E-21 | 8.56E-01 | 1.19E-01 | 1.49E-02 | 1.02E-02 |
| 5.80E+01 | 2.96E-232 | 8.56E-56 | 8.65E-20 | 1.22E-22 | 1.20E-14 | 2.10E-21 | 8.55E-01 | 1.20E-01 | 1.49E-02 | 1.02E-02 |
| 5.90E+01 | 3.09E-238 | 2.21E-57 | 2.67E-20 | 2.50E-23 | 5.41E-15 | 4.74E-22 | 8.53E-01 | 1.21E-01 | 1.51E-02 | 1.03E-02 |
| 6.00E+01 | 3.24E-244 | 5.70E-59 | 8.23E-21 | 5.13E-24 | 2.44E-15 | 1.07E-22 | 8.51E-01 | 1.24E-01 | 1.53E-02 | 1.04E-02 |
| 6.10E+01 | 3.40E-250 | 1.47E-60 | 1.85E-21 | 1.05E-24 | 1.10E-15 | 2.42E-23 | 8.46E-01 | 1.28E-01 | 1.58E-02 | 1.07E-02 |
| 6.20E+01 | 3.59E-256 | 3.78E-62 | 4.15E-22 | 2.17E-25 | 4.89E-16 | 5.47E-24 | 8.37E-01 | 1.35E-01 | 1.67E-02 | 1.14E-02 |
| 6.30E+01 | 3.81E-262 | 9.66E-64 | 9.29E-23 | 4.44E-26 | 2.15E-16 | 1.23E-24 | 8.22E-01 | 1.46E-01 | 1.86E-02 | 1.28E-02 |
| 6.40E+01 | 4.07E-268 | 2.45E-65 | 2.04E-23 | 8.94E-27 | 9.17E-17 | 2.74E-25 | 7.96E-01 | 1.65E-01 | 2.23E-02 | 1.59E-02 |
| 6.50E+01 | 4.45E-274 | 6.10E-67 | 4.14E-24 | 1.68E-27 | 3.63E-17 | 5.67E-26 | 7.53E-01 | 1.95E-01 | 2.96E-02 | 2.28E-02 |

A-5.4.4. TPFQ Profile for COL-302

| Stage | Temperature | Pressure | Heat duty | Liquid from (Mass) | Vapor from (Mass) | Liquid enthalpy | Vapor enthalpy | Liquid flow (Mass) | Vapor flow (Mass) |
|---|---|---|---|---|---|---|---|---|---|
| | F | psia | Btu/hr | lb/hr | lb/hr | Btu/lbmol | Btu/lbmol | lb/hr | lb/hr |
| 1 | 196 | 16.0 | -33077660 | 187342 | 0 | 19206 | 34800 | 73224 | 0 |
| 2 | 241 | 26.0 | 0 | 80177 | 187342 | 17010 | 33997 | 80177 | 187342 |
| 3 | 251 | 26.2 | 0 | 80163 | 194294 | 14667 | 32850 | 80163 | 194294 |
| 4 | 258 | 26.3 | 0 | 80114 | 194281 | 13201 | 32115 | 80114 | 194281 |
| 5 | 262 | 26.5 | 0 | 80008 | 194232 | 12272 | 31673 | 80008 | 194232 |
| 6 | 265 | 26.6 | 0 | 79878 | 194126 | 11661 | 31406 | 79878 | 194126 |
| 7 | 267 | 26.8 | 0 | 79739 | 193996 | 11243 | 31239 | 79739 | 193996 |
| 8 | 268 | 26.9 | 0 | 79595 | 193857 | 10938 | 31130 | 79595 | 193857 |
| 9 | 270 | 27.1 | 0 | 79440 | 193713 | 10698 | 31057 | 79440 | 193713 |
| 10 | 271 | 27.2 | 0 | 79269 | 193558 | 10483 | 31003 | 79269 | 193558 |
| 11 | 272 | 27.4 | 0 | 79073 | 193387 | 10268 | 30958 | 79073 | 193387 |
| 12 | 273 | 27.5 | 0 | 78846 | 193191 | 10028 | 30916 | 78846 | 193191 |
| 13 | 274 | 27.7 | 0 | 78578 | 192963 | 9744 | 30869 | 78578 | 192963 |
| 14 | 275 | 27.8 | 0 | 78266 | 192696 | 9400 | 30815 | 78266 | 192696 |
| 15 | 276 | 28.0 | 0 | 77905 | 192384 | 8984 | 30748 | 77905 | 192384 |
| 16 | 278 | 28.1 | 0 | 77499 | 192023 | 8490 | 30667 | 77499 | 192023 |
| 17 | 280 | 28.3 | 0 | 77053 | 191617 | 7919 | 30570 | 77053 | 191617 |
| 18 | 281 | 28.4 | 0 | 76584 | 191171 | 7282 | 30458 | 76584 | 191171 |
| 19 | 284 | 28.6 | 0 | 76109 | 190701 | 6601 | 30334 | 76109 | 190701 |
| 20 | 286 | 28.7 | 0 | 75663 | 190227 | 5906 | 30202 | 75663 | 190227 |
| 21 | 288 | 28.9 | 0 | 75506 | 189781 | 5237 | 30066 | 75506 | 189781 |
| 22 | 289 | 29.0 | 0 | 80889 | 189623 | 4741 | 29908 | 80889 | 189623 |
| 23 | 288 | 29.2 | 0 | 163448 | 150403 | 5160 | 26970 | 163448 | 150403 |
| 24 | 315 | 29.3 | 0 | 169477 | 151735 | 330 | 21912 | 169477 | 151735 |
| 25 | 337 | 29.5 | 0 | 176292 | 157765 | -3111 | 17144 | 176292 | 157765 |
| 26 | 352 | 29.6 | 0 | 181972 | 164579 | -5301 | 13515 | 181972 | 164579 |
| 27 | 363 | 29.8 | 0 | 185912 | 170259 | -6669 | 11098 | 185912 | 170259 |

| Stage | Temperature | Pressure | Heat duty | Liquid from (Mass) | Vapor from (Mass) | Liquid enthalpy | Vapor enthalpy | Liquid flow (Mass) | Vapor flow (Mass) |
|---|---|---|---|---|---|---|---|---|---|
| 28 | 369 | 29.9 | 0 | 188453 | 174199 | -7543 | 9561 | 188453 | 174199 |
| 29 | 374 | 30.1 | 0 | 190093 | 176740 | -8118 | 8581 | 190093 | 176740 |
| 30 | 377 | 30.2 | 0 | 191189 | 178381 | -8503 | 7941 | 191189 | 178381 |
| 31 | 379 | 30.4 | 0 | 191953 | 179476 | -8764 | 7513 | 191953 | 179476 |
| 32 | 380 | 30.5 | 0 | 192507 | 180240 | -8940 | 7223 | 192507 | 180240 |
| 33 | 382 | 30.7 | 0 | 192923 | 180794 | -9058 | 7025 | 192923 | 180794 |
| 34 | 383 | 30.8 | 0 | 193248 | 181211 | -9134 | 6891 | 193248 | 181211 |
| 35 | 384 | 31.0 | 0 | 193508 | 181535 | -9182 | 6800 | 193508 | 181535 |
| 36 | 384 | 31.1 | 0 | 193722 | 181795 | -9208 | 6741 | 193722 | 181795 |
| 37 | 385 | 31.3 | 0 | 193905 | 182010 | -9219 | 6704 | 193905 | 182010 |
| 38 | 385 | 31.4 | 0 | 194065 | 182193 | -9220 | 6683 | 194065 | 182193 |
| 39 | 386 | 31.6 | 0 | 194208 | 182352 | -9213 | 6673 | 194208 | 182352 |
| 40 | 386 | 31.7 | 0 | 194340 | 182496 | -9201 | 6672 | 194340 | 182496 |
| 41 | 387 | 31.9 | 0 | 194453 | 182627 | -9185 | 6676 | 194453 | 182627 |
| 42 | 387 | 32.0 | 24137701 | 11713 | 182741 | -9168 | 6686 | 11713 | 182741 |

A-5.4.5. Liquid Mass Composition Profile for COL-302

| Stage | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|
| 1 | 0.616 | 0.304 | 0.080 | 0.000 |
| 2 | 0.420 | 0.399 | 0.180 | 0.001 |
| 3 | 0.314 | 0.416 | 0.267 | 0.002 |
| 4 | 0.263 | 0.398 | 0.335 | 0.004 |
| 5 | 0.238 | 0.372 | 0.384 | 0.006 |
| 6 | 0.225 | 0.348 | 0.418 | 0.009 |
| 7 | 0.218 | 0.329 | 0.440 | 0.012 |
| 8 | 0.214 | 0.316 | 0.453 | 0.017 |
| 9 | 0.211 | 0.306 | 0.460 | 0.024 |
| 10 | 0.208 | 0.298 | 0.461 | 0.032 |
| 11 | 0.206 | 0.292 | 0.459 | 0.042 |
| 12 | 0.204 | 0.287 | 0.452 | 0.056 |
| 13 | 0.202 | 0.282 | 0.443 | 0.073 |
| 14 | 0.200 | 0.276 | 0.430 | 0.095 |
| 15 | 0.197 | 0.270 | 0.413 | 0.120 |
| 16 | 0.193 | 0.262 | 0.393 | 0.151 |
| 17 | 0.189 | 0.254 | 0.370 | 0.186 |
| 18 | 0.185 | 0.245 | 0.345 | 0.224 |
| 19 | 0.180 | 0.236 | 0.318 | 0.265 |
| 20 | 0.176 | 0.227 | 0.291 | 0.306 |
| 21 | 0.171 | 0.218 | 0.265 | 0.346 |
| 22 | 0.169 | 0.211 | 0.241 | 0.378 |
| 23 | 0.170 | 0.234 | 0.225 | 0.371 |
| 24 | 0.075 | 0.173 | 0.252 | 0.500 |
| 25 | 0.028 | 0.108 | 0.243 | 0.620 |
| 26 | 0.010 | 0.061 | 0.211 | 0.718 |
| 27 | 0.003 | 0.032 | 0.172 | 0.793 |
| 28 | 0.001 | 0.016 | 0.134 | 0.849 |
| 29 | 0.000 | 0.008 | 0.102 | 0.890 |
| 30 | 0.000 | 0.004 | 0.076 | 0.920 |
| 31 | 0.000 | 0.002 | 0.056 | 0.942 |
| 32 | 0.000 | 0.001 | 0.041 | 0.958 |
| 33 | 0.000 | 0.000 | 0.030 | 0.970 |
| 34 | 0.000 | 0.000 | 0.022 | 0.978 |
| 35 | 0.000 | 0.000 | 0.016 | 0.984 |
| 36 | 0.000 | 0.000 | 0.011 | 0.989 |
| 37 | 0.000 | 0.000 | 0.008 | 0.992 |
| 38 | 0.000 | 0.000 | 0.006 | 0.994 |
| 39 | 0.000 | 0.000 | 0.004 | 0.996 |
| 40 | 0.000 | 0.000 | 0.003 | 0.997 |
| 41 | 0.000 | 0.000 | 0.002 | 0.998 |

| Stage | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|
| 42 | 0.000 | 0.000 | 0.001 | 0.999 |

A-5.4.6. Vapor Mass Composition Profile for COL-302

| Stage | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|
| 1 | 0.744 | 0.216 | 0.040 | 0.000 |
| 2 | 0.616 | 0.304 | 0.080 | 0.000 |
| 3 | 0.535 | 0.343 | 0.121 | 0.001 |
| 4 | 0.491 | 0.350 | 0.157 | 0.001 |
| 5 | 0.470 | 0.343 | 0.185 | 0.002 |
| 6 | 0.460 | 0.332 | 0.205 | 0.003 |
| 7 | 0.455 | 0.322 | 0.219 | 0.004 |
| 8 | 0.452 | 0.314 | 0.228 | 0.005 |
| 9 | 0.451 | 0.309 | 0.233 | 0.007 |
| 10 | 0.449 | 0.305 | 0.236 | 0.010 |
| 11 | 0.449 | 0.302 | 0.236 | 0.013 |
| 12 | 0.448 | 0.299 | 0.235 | 0.018 |
| 13 | 0.448 | 0.297 | 0.232 | 0.023 |
| 14 | 0.447 | 0.295 | 0.228 | 0.030 |
| 15 | 0.447 | 0.293 | 0.222 | 0.039 |
| 16 | 0.446 | 0.290 | 0.215 | 0.049 |
| 17 | 0.445 | 0.287 | 0.207 | 0.061 |
| 18 | 0.444 | 0.284 | 0.197 | 0.075 |
| 19 | 0.443 | 0.280 | 0.187 | 0.090 |
| 20 | 0.442 | 0.277 | 0.175 | 0.106 |
| 21 | 0.440 | 0.273 | 0.164 | 0.122 |
| 22 | 0.439 | 0.270 | 0.154 | 0.138 |
| 23 | 0.342 | 0.279 | 0.181 | 0.198 |
| 24 | 0.183 | 0.252 | 0.243 | 0.322 |
| 25 | 0.080 | 0.185 | 0.271 | 0.463 |
| 26 | 0.030 | 0.116 | 0.260 | 0.593 |
| 27 | 0.010 | 0.065 | 0.226 | 0.699 |
| 28 | 0.003 | 0.034 | 0.183 | 0.779 |
| 29 | 0.001 | 0.017 | 0.143 | 0.839 |
| 30 | 0.000 | 0.008 | 0.108 | 0.883 |
| 31 | 0.000 | 0.004 | 0.081 | 0.915 |
| 32 | 0.000 | 0.002 | 0.059 | 0.939 |
| 33 | 0.000 | 0.001 | 0.043 | 0.956 |
| 34 | 0.000 | 0.000 | 0.032 | 0.968 |
| 35 | 0.000 | 0.000 | 0.023 | 0.977 |
| 36 | 0.000 | 0.000 | 0.016 | 0.983 |
| 37 | 0.000 | 0.000 | 0.012 | 0.988 |

| Stage | Benzene | Toluene | Xylene | Trimethylbenzene |
|---|---|---|---|---|
| 38 | 0.000 | 0.000 | 0.008 | 0.992 |
| 39 | 0.000 | 0.000 | 0.006 | 0.994 |
| 40 | 0.000 | 0.000 | 0.004 | 0.996 |
| 41 | 0.000 | 0.000 | 0.003 | 0.997 |
| 42 | 0.000 | 0.000 | 0.002 | 0.998 |

## A-6. Consultant E-mail Correspondence

### *A-6.1. Ms. Karin Fair, Air Products and Chemicals, Inc.*

---------- Forwarded message ----------
From: **Fair,Karin Aurora** <FAIRKA@airproducts.com>
Date: Mon, Mar 23, 2015 at 10:41 PM
Subject: RE: PRISM Separation
To: Arthur Chen <arthurchen24@gmail.com>

Hello, Arthur.

Answers are in your e-mail below.

Regards,
Karin Fair

**From:** Arthur Chen [mailto:arthurchen24@gmail.com]
**Sent:** Sunday, March 22, 2015 1:08 PM
**To:** Fair,Karin Aurora
**Subject:** Re: PRISM Separation

Hi Karin,

Thank you so much for the help. We just had a couple of followup questions as we complete our project.

1) Are there any temperature considerations for the separation at 1200 psig?
With operating at either feed pressure of 700 psig or 1200 psi, typical operating pressure for feed gas containing H2 and hydrocarbons is 83°C. Typical pretreatment is cooler (if feed gas temperature is more than about 45°C) to cool to 40°C, mist eliminator to remove condensed liquids, and feed heater to superheat the feed gas to 83°C.
2) What are the outlet pressures for the permeate and diffusate in the same 1200 psig case?
The permeate (H2-rich / fast gas) stream is 200 psig. The non-permeate (HC-rich / slower gas) stream would be at about 1150 psig and then can be let down to a lower pressure if necessary.
3) Is PRISM suitable for a second further separation of methane? Such a separation would be looking to achieve ethane purity.
Are you asking if the membrane can be used to separate methane from ethane and the other HC's? If so, the answer is no. There is not enough difference between the C1 and C2 component permeabilities to make that an effective separation.
4) Lastly, about how much would such a piece of equipment cost?
I think the MW of the feed gas is 16.21 kg/kgmole. So for 135,000 kg/hr feed flow rate, that means 8333 kmol/hr or 167 MMSCFD. This is a large feed flow, and given the low purity feed gas (only 42 mol% H2), I'm not so sure that a membrane is the most economic solution. For 8333 kmol/hr, 700 psig feed, 200 psig permeate, a rough cost for the membrane system is $17MM (17 million dollars).

Also some added information: we are using a feed flow rate of 1.35 x 10^5 kg/hr and a pressure of 700 psig.

Thank you in advance for your kind advice.

Best,
Arthur

On Mon, Mar 2, 2015 at 11:33 PM, Fair,Karin Aurora <FAIRKA@airproducts.com> wrote:
Hello,

The higher level of aromatics in the right-hand composition could be problematic, so would likely be better for the membrane to have heavy HC's removed upstream of the membranes. Here are some general comments:

- Membranes use partial pressure as the driving force for the separation. Feed is at higher pressure. Permeate (H2-rich) is at lower pressure.

- If feed is at 700 psig and permeate is at 200 psig, with targeting 85% recovery, expected permeate purity is about 72 mol% H2.

- If feed is at 1200 psig and permeate is at 200 psig, with targeting 85% recovery, expected permeate purity is about 81 mol% H2.

- Higher H2 recovery results in lower H2 purity permeate.

You didn't specify either a H2 recovery or a H2 purity that you're looking to achieve, so not sure if the recovery and/or purity that I report above is close to what you're expecting.

-Karin

**From:** Arthur Chen [mailto:arthurchen24@gmail.com]
**Sent:** Monday, March 02, 2015 3:57 PM
**To:** Fair,Karin Aurora
**Subject:** Re: PRISM Separation

Thank you for your quick reply.

Depending on the placement of the membrane separation in our process, there are two possible feed compositions (on left: after separation of heavy hydrocarbons; on right: before separation).

| Mole Frac | | |
|---|---|---|
| HYDROGEN | 0.421367 | 0.3868498 |
| METHANE | 0.1507092 | 0.139271 |
| ETHANE | 0.3714968 | 0.3478525 |
| ETHYLENE | 0.0422207 | 0.0393063 |

| | | |
|---|---|---|
| PROPANE | 0.00977494 | 0.010147 |
| PROPYLENE | 0.0034205 | 0.00329065 |
| BENZENE | 0.000996064 | 0.0453434 |
| TOLUENE | 1.46E-05 | 0.0187711 |
| P-XYLENE | 9.53E-08 | 0.00429653 |
| TRIMETHYLBENZENE | 2.20E-09 | 0.0048715 |

The feed gas pressure and temperature are flexible, as we have yet to set those conditions in stone. The same goes for the permeate stream. As for the performance we wish to achieve, it is H2 recovery.

Again, all your help is deeply appreciated.

Best,
Arthur Chen

On Mon, Mar 2, 2015 at 11:04 AM, Fair,Karin Aurora <FAIRKA@airproducts.com> wrote:
Hello,

I have some questions in order to assess if a membrane is a viable technology for you.

- Can you please provide a more complete feed composition?  The composition you provided (H2, C1, other products) only adds up to 0.882.
- What is the feed flow rate?
- What is the feed gas pressure?
- What pressure do you need the permeate (H2-rich) stream?
- What performance are you wanting to achieve – either H2 recovery and/or permeate H2 purity?

Regards,
Karin Fair

**From:** Arthur Chen [mailto:arthurchen24@gmail.com]
**Sent:** Monday, March 02, 2015 10:35 AM
**To:** Fair,Karin Aurora
**Subject:** PRISM Separation

Dear Karin Fair,

Good morning. I am writing to you on behalf of my chemical engineering senior design team. We received your contact information from our classmates on another team.

Our project has some similarities to theirs, namely in that we have a stream with a mixture of hydrogen and light hydrocarbons from which we wish to separate out the hydrogen for sale or other use. Specifically, our stream had a composition of 0.389 hydrogen, 0.130 methane, and 0.363 plus small quantities of other products.

We are hoping that you could provide some insight as to what specific PRISM conditions we would theoretically require to separate out our hydrogen, and how much that would cost. Furthermore, we are curious if PRISM can separate methane as well. Any suggestions or insight you can provide would be greatly appreciated.

Best regards,
Arthur Chen

### *A-6.2. Ms. Sasha Maitala, Jacobs UK*

---------- Forwarded message ----------
From: "Maitala, Sasha" <Sasha.Maitala@jacobs.com>
Date: Mon, 30 Mar 2015 16:40:37 +0100
Subject: Steam Reformer Reactor
To: "crowleyf@seas.upenn.edu" <crowleyf@seas.upenn.edu>

Hi Fiona,

I have been asked to provide you with some information for your senior design project.

If you go with a steam reformer type reactor unit you should know that it has a significant amount of heat that can and should be recovered from the flue gas. The temperature you have specified is a little low for typical steam reformer duties but a solution could be easily found.

The total installed cost of a steam reformer with the absorbed heat duty you have quoted is in the region of 55 million USD. The price includes the heat recovery section of the reactor.

The footprint of the reactor with the heat recovery section and all civil/structural works is:
29 m Length
18 m Width
32 m Height to top of penthouse roof (not including stack height)

Attached is a picture of an existing reformer. Your unit will be roughly twice the twice of that one.

Hope you find this information helpful,

Regards,
Sasha

Sasha Maitala | Jacobs | Process Engineer | +44 (0) 20 7378 2841 |
sasha.maitala@jacobs.com<mailto:sasha.maitala@jacobs.com> |
www.jacobs.com
<http://www.jacobs.com/

>

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### *A-6.3. Dr. Richard Bockrath, DuPont*

---------- Forwarded message ----------
From: **Richard Bockrath** <richardbockrath@gmail.com>
Date: Wed, Apr 1, 2015 at 6:36 AM
Subject: Re: BTX from Ethane: Steam Boiler
To: Arthur Chen <arthurchen24@gmail.com>

Attached is the boiler info I have. The boiler is sized for about 50% of your steam generation rates so you would need two of these boilers. We had talked about the value of having two boilers anyways and so this is probably a good size for your work. Our engineering firm said this was "a small boiler for a refinery or petrochemical plant". The price was for January, 2014 and so you would need to adjust it for inflation from then to when you would buy it for your plant. The pressure rating is lower than you desire. I am not sure if the database you are currently using shows the price impact of different output pressures in its tables. If it doesn't then I would just add 10% to the price in the attachment for higher output pressure.

Hope this helps. Let me know if you need more.

Rick

On Tue, Mar 31, 2015 at 10:25 PM, Arthur Chen <arthurchen24@gmail.com> wrote:
Hi Dr. Bockrath,

Just wanted to follow up on our meeting this afternoon. We mentioned that we needed a steam boiler that could handle a heat requirement of 254 million BTU/hr. You mentioned that you were working with on a project with a similar large steam boiler and may have some information on the sizing and cost of such a unit.

Thanks,
Arthur

## 15. Steam Boiler

The steam demand requirements were based on the Processium energy balance and the design basis is listed in Table 22. The assumed steam pressure is 100 psig to provide sufficient temperature differential to meet maximum reboiler temperatures. The temperatures in the Processium material balance are subject to change based on results during pilot plant operation.

One vendor was contacted for a budgetary estimate for the steam boiler and a summary of the proposal is provided in Table 23.

**Table 22. Steam Boiler Design Basis**

| *Parameter* | *Value* | *Comments* |
|---|---|---|
| Steam Supply Pressure | 100 psig | Based on maximum estimated reboiler temperatures in Processium energy balance |
| Steam Demand | 165,000 lb/hr | Based on Processium steady state energy balance and GBE fermentation CIP process |

**Table 23. Summary of Steam Boiler Vendor Estimate**

| | |
|---|---|
| *Vendor* | Babcock and Wilcox |
| *Boiler Capacity* | 165,000 lb/hr |
| *Produced Steam Pressure* | 100 psig |
| *Produced Steam Temperature* | Saturated |
| *Boiler Package* | FM120-112 Water Tube |
| *Pricing FOB point of fabrication* | $1,387,300 |

Fisher Scientific sells at lab scale and so their price will be far too high. Alibaba is an industrial eBay for China. They always low ball their prices. I would pick something between the two. I would guess it is more like $10-15/kg. Say $12.5/kg.

Rick

On Apr 4, 2015 5:05 PM, "Jonathan Lym" <jlym@seas.upenn.edu> wrote:
Hi Dr. Bockrath,

That's good news to hear! Thank you!

Sorry to barrage you with more questions but we were talking to another group about the price of ZSM-5 and found that we were using two completely different values.

Our estimate was $92.2 per kg from Fisher Scientific but their group's estimate was $4.9 per kg from Alibaba. Which cost do you think is more reasonable?

Thank you again for all the help you've provided.

Sincerely,
Jon

--
**Jonathan Lym**
School of Engineering and Applied Sciences
University of Pennsylvania, Class of 2015
M: (909) 451- 1777 | jlym@seas.upenn.edu

On Fri, Apr 3, 2015 at 11:43 AM, Richard Bockrath <richardbockrath@gmail.com> wrote:

Praxair and Linde both have numerous pipelines in the Texas petrochemical hub. If you dig a hole in that area you will probably break a pipe! So I think it is quite reasonable to assume you can get hydrogen, N2 and O2 from them. Chlorine is stored in carbon steel pressurized tanks. Its vapor pressure is low enough that the pressure rating on the tank is very reasonable. This is Texas and so assume the tank will be exposed to the heat of the summer ie the pressure rating must be able to handle Cl2 at 50oC. So on site storage is the norm. People try to store as little Cl2 as possible due to permitting issues. So I would size the tank to either a) hold one smaller rail car of Cl2 (This would be about 80,000 lb of Cl2) or b) one week of usage whichever is larger.

Good luck and it has been a pleasure working with you all.

Rick

Hi Dr. Bockrath,

Firstly I want to say thank you so much for your help. We have made significant progress with your help.

We had found the flowrates required for the regeneration process but now our group was discussing the sources of the gases (i.e. chlorine, nitrogen, hydrogen and oxygen). We found this website
on Praxair's website that says it has pipelines available on the Gulf Coast for nitrogen, hydrogen and oxygen.

Do you see any issues with using these pipelines for our process? Also we were planning on storing chlorine on site in a pressure vessel. Is this standard for an industrial plant?

Thank you again for the guidance!

Best,
Jon
--

Yes you should assume fractionation grade. I would just guess it is 1% methane, 97% ethane and 2% propane.

Rick

Hi Dr. Bockrath,

Sorry about the late response. I had fallen asleep. I had initially got that information from the US Department of Transportation
and some pages in a book called the Fundamentals of Natural Gas Processing. Upon further examination of the chapter, I found this is a figure that gives a more accurate composition of liquid products (see page 141 of the book available here
):

Could we then assume we're using Fractionation grade ethane?

Best,
Jon