

PRODUCTION OF BTX FROM ETHANE

Design Project By:

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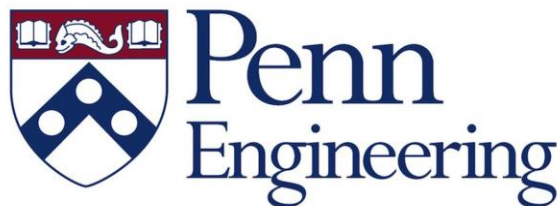
Presented To:

Professor Leonard Fabiano
Dr. Daeyeon Lee

April 14, 2015

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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°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,

A handwritten signature in black ink, appearing to read "Arthur Chen".

Arthur Chen

A handwritten signature in black ink, appearing to read "Fiona Crowley".

Fiona Crowley

A handwritten signature in black ink, appearing to read "Jonathan Lym".

Jonathan Lym

A handwritten signature in black ink, appearing to read "Pablo Sanchez".

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.

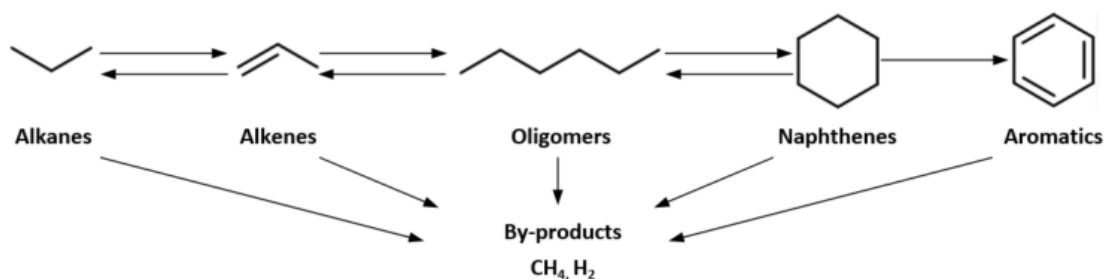


Figure 1. General mechanism for the aromatization of alkanes¹.

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 found². 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 209,795³ and US Patent 324,778⁴.

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	ΔH_{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°F.

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.

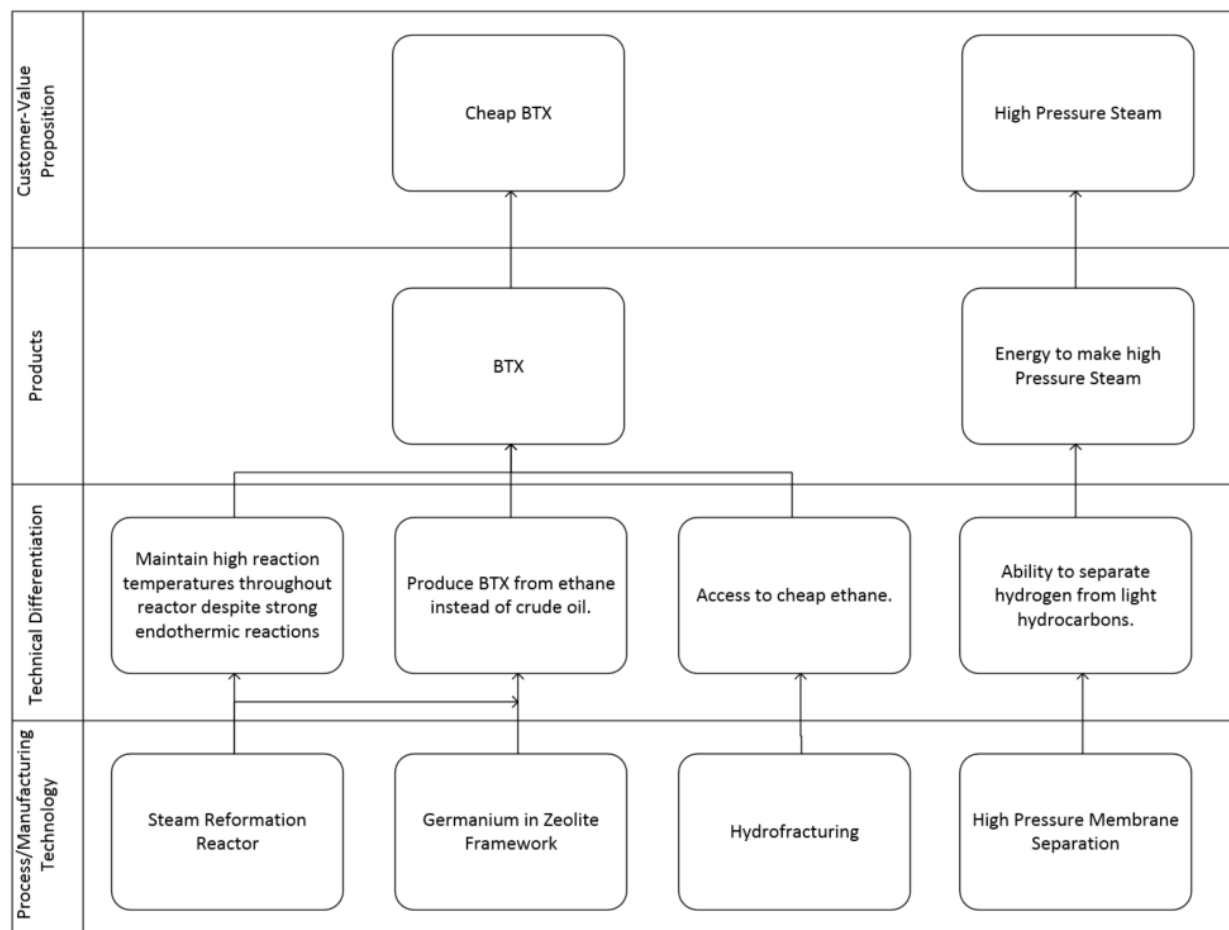


Figure 2. Innovation Map for the Proposed Process Design.

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 feet⁵. 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.

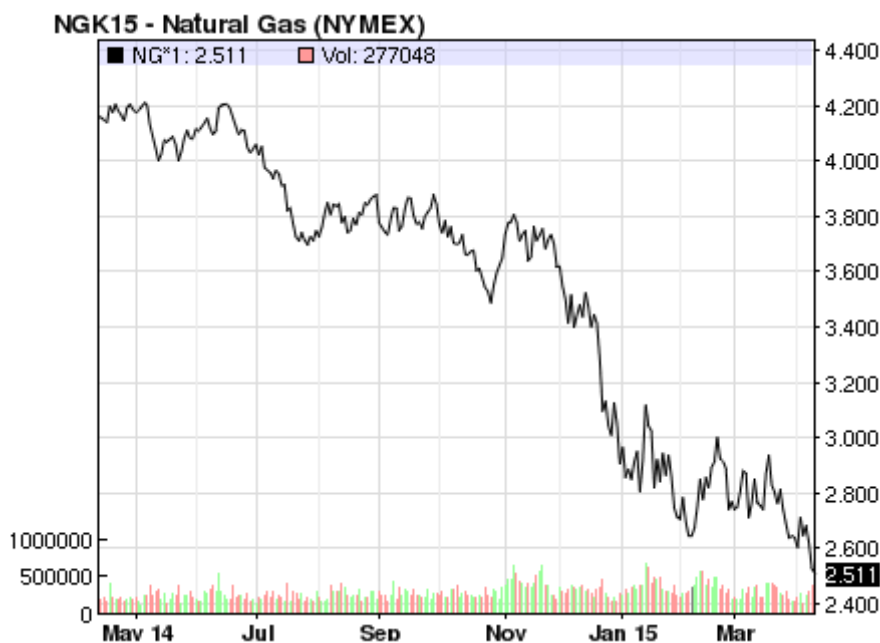
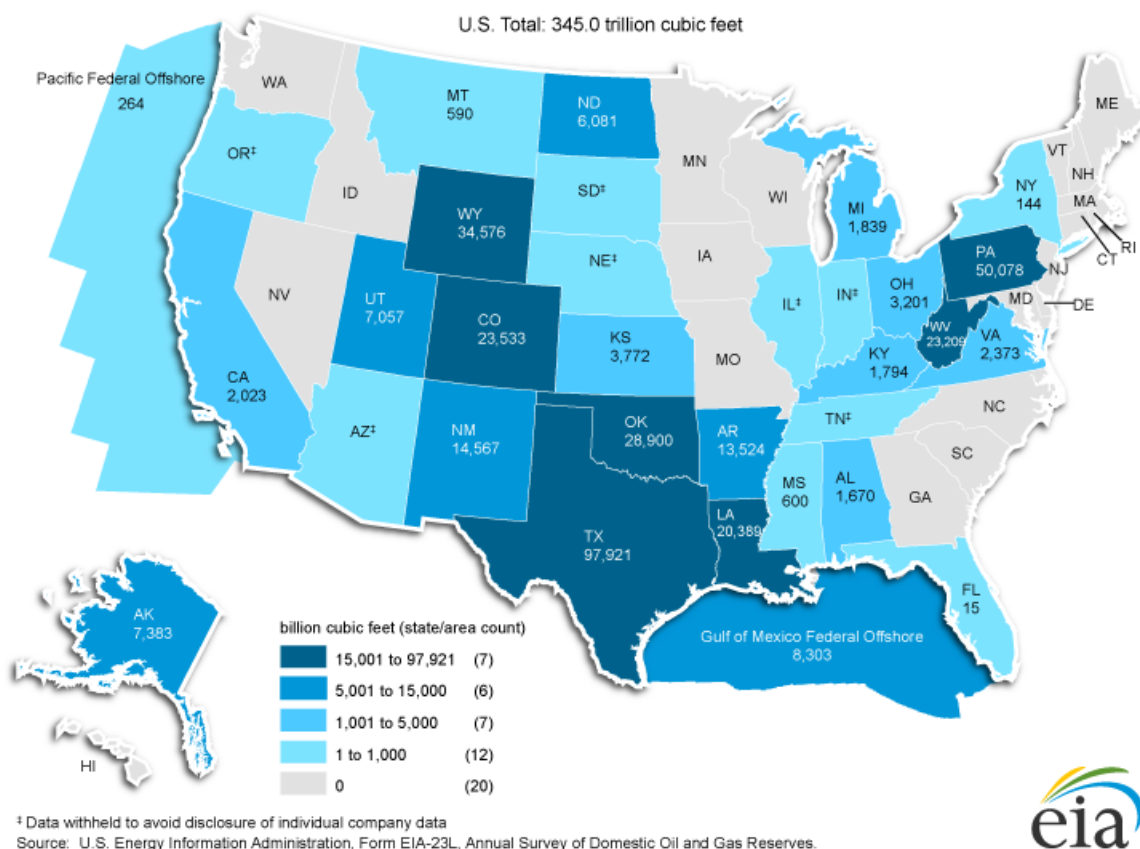


Figure 3. Natural gas prices from April 2014 to April 2015⁵.



Figure 4. Ethane spot prices (per gallon) from December 2014 to April 2015⁵.

Figure 5. Natural gas proved reserves by sales/area, 2013⁵

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 regulated²⁶. 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 209,795³, 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 324,778⁴, 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 209,795³, 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 209,795³ 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 324,778⁴ 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 154,079⁶, 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 alumina⁷. 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.

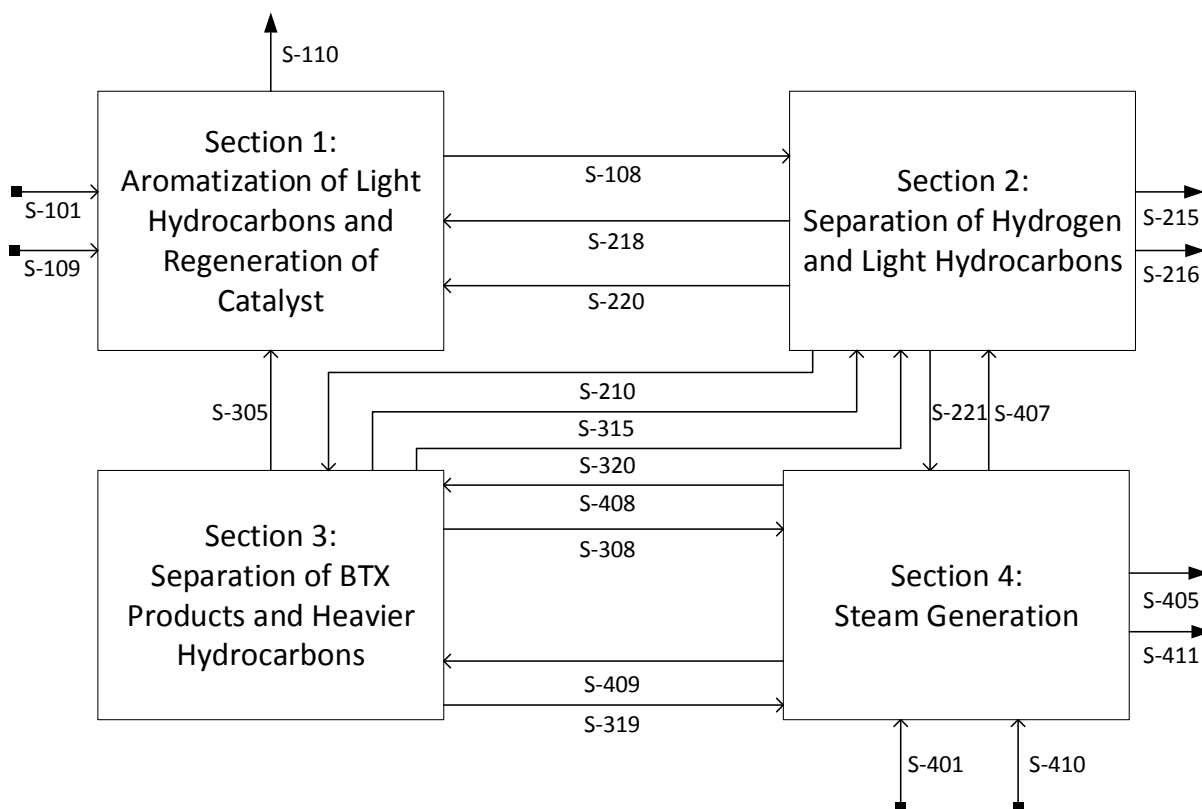


Figure 6. Overview of the interactions among the four different sections of the process.

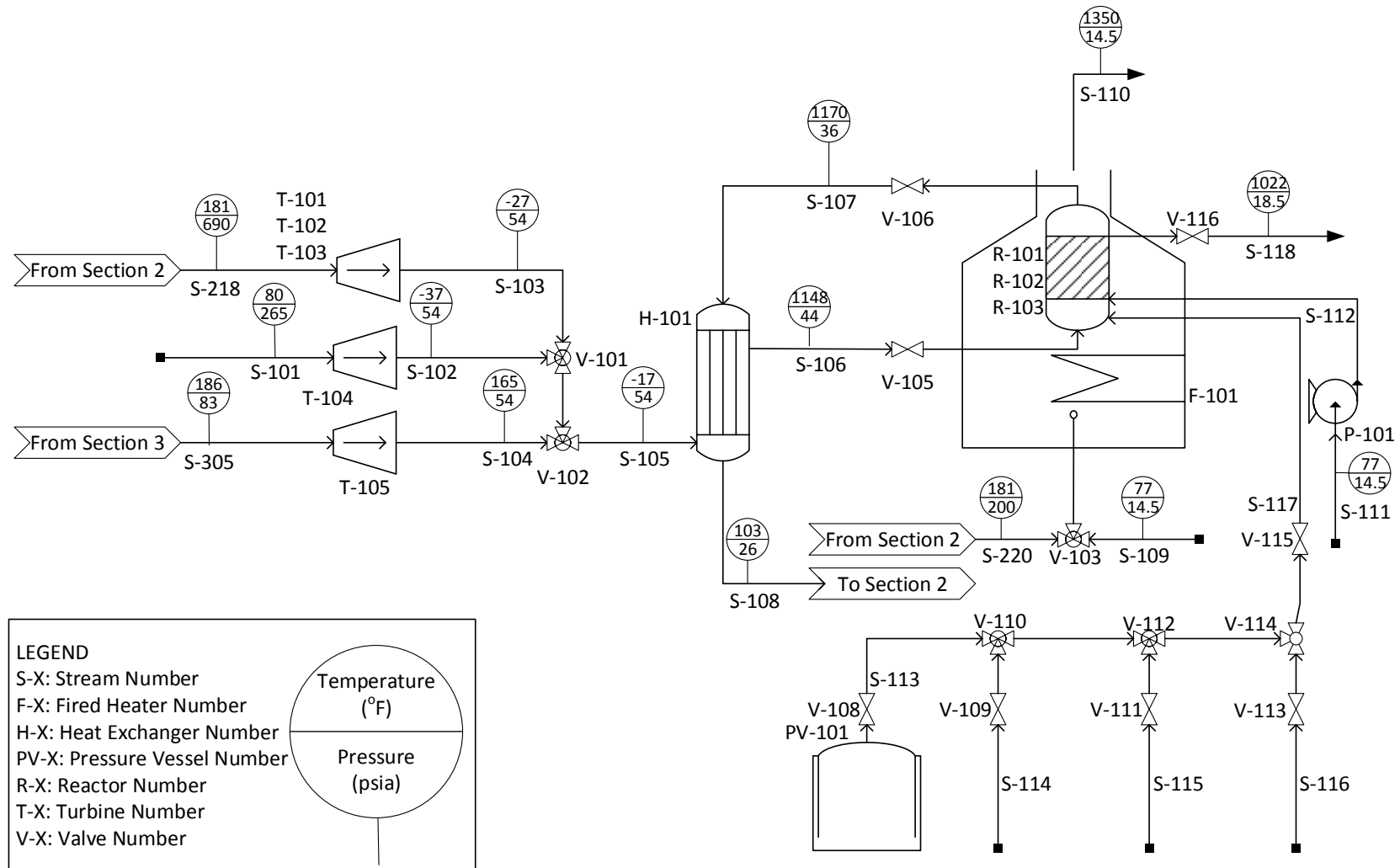


Figure 7. Section 1: Aromatization of Light Hydrocarbons and Regeneration of Catalyst

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.

Species	Mass Flow (lb/hr)									
	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 (°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

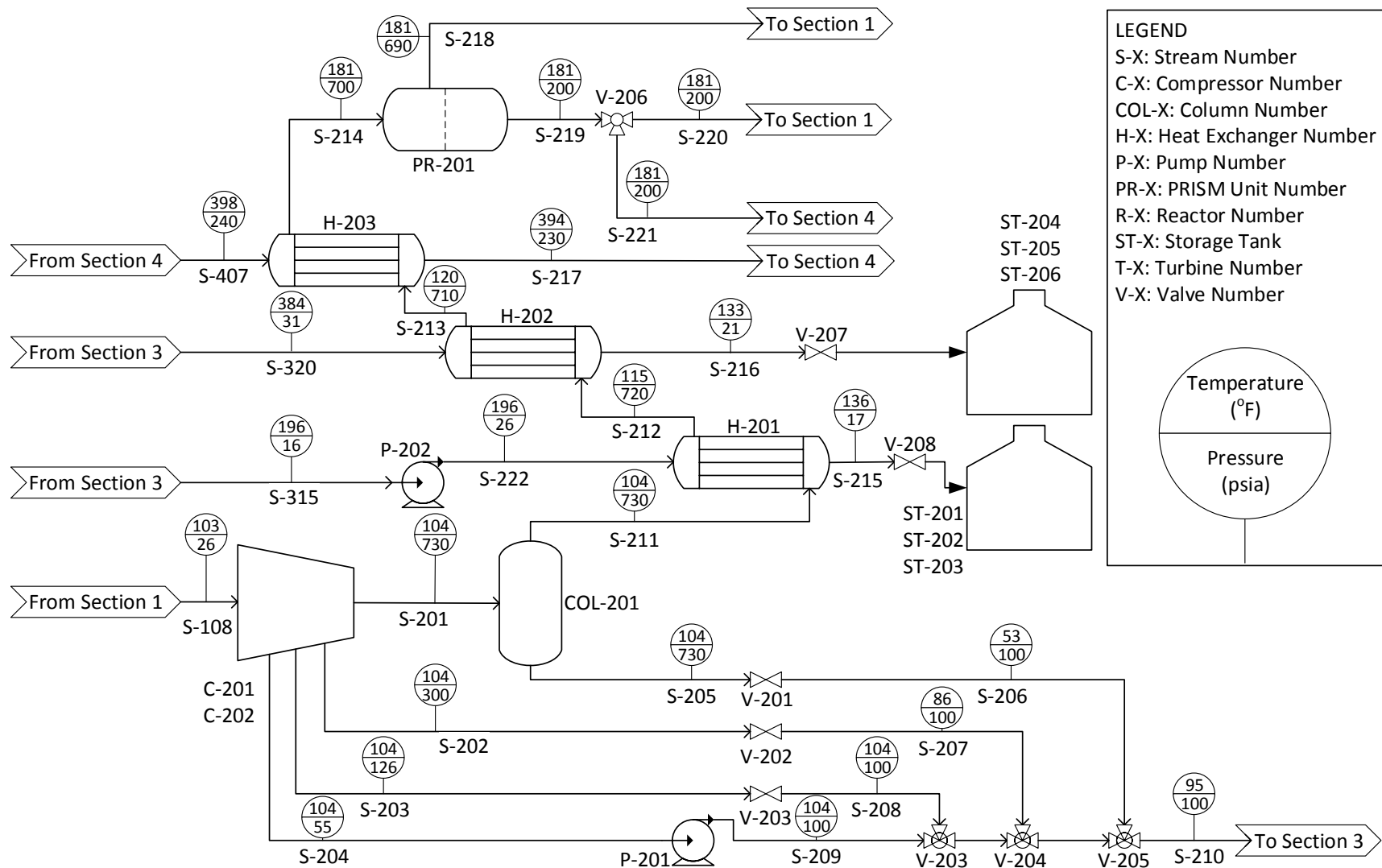


Figure 8. Section 2: Separation of Hydrogen and Light Hydrocarbons

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.

Species	Mass Flow (lb/hr)									
	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 (°F)	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.

Species	Mass Flow (lb/hr)									
	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 (°F)	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 (°F)	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

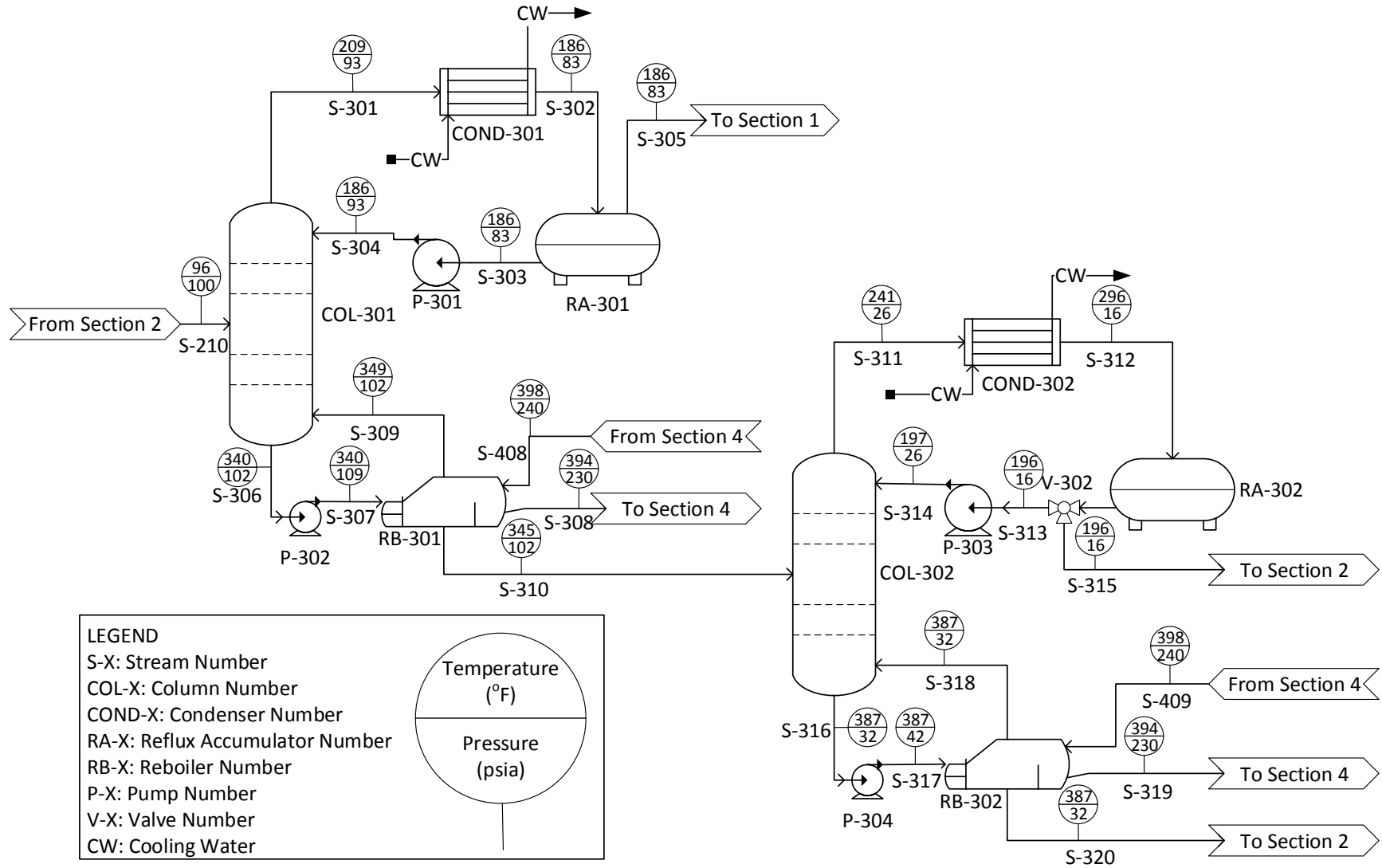


Figure 9. Section 3: Separation of BTX Products and Heavier Hydrocarbons

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.

Species	Mass Flow (lb/hr)									
	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 (°F)	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.

Species	Mass Flow (lb/hr)									
	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 (°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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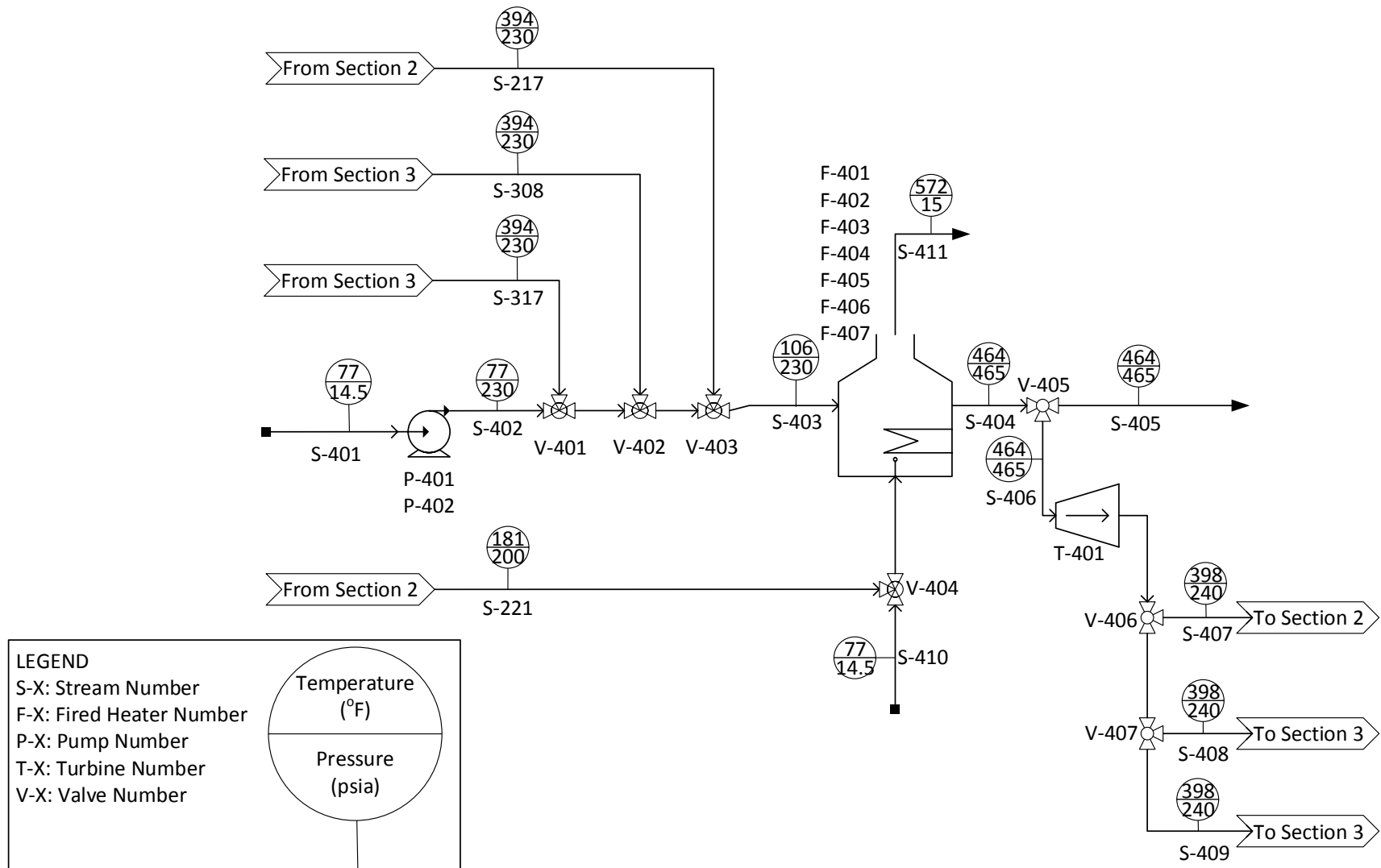


Figure 10. Section 4: Steam Generation

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.

Species	Mass Flow (lb/hr)									
	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 (°F)	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.

Species	Mass Flow (lb/hr)
	S-411
Water	198009
Oxygen	49890
Nitrogen	985838
Carbon Dioxide	101223
Total Flow (lb/hr)	1334960
Total Flow (cuft/hr)	38194900
Temperature (°F)	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% propane¹⁸, enters the process through available pipelines along the Gulf Coast at a temperature of 88°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°F to 1148°F.

Aromatization

The preheated stream, S-106, then enters the furnace where it is heated to 1170°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°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 209,795² 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 324,778³. 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°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°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 (°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.

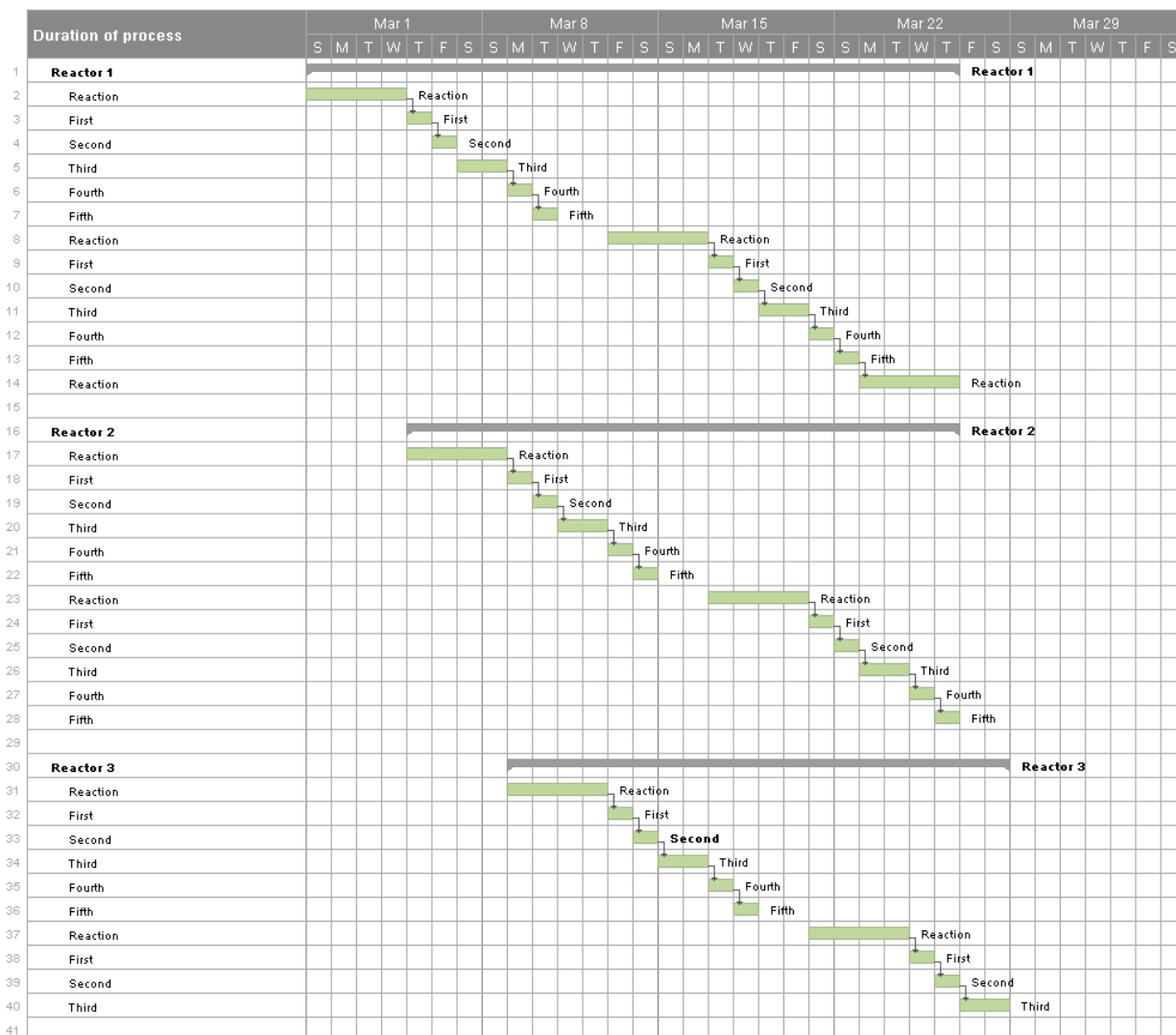


Figure 11. Gantt chart for the regeneration process. ‘Reaction’ represents the period in which the reactor is in operation. ‘First’, ‘Second’, ‘Third’, ‘Fourth’, and ‘Fifth’ represent the different stages of the regeneration process.²⁰

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 °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°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°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°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°F. The hot stream exits at 133°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°F to be fed into the final shell and tube heat exchanger, H-203. This heat exchanger heats the gas to 181°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°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°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°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°F and a pressure of 26 psia. Stream S-311 passes through a total condenser where it is cooled to a temperature of 200°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°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°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°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°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°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°F. F-101 will allow S-106 to reach the operating temperature of 1350°F and keep the reactors at an isothermal temperature of 1350°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°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 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 T-102 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 Principles¹⁴.

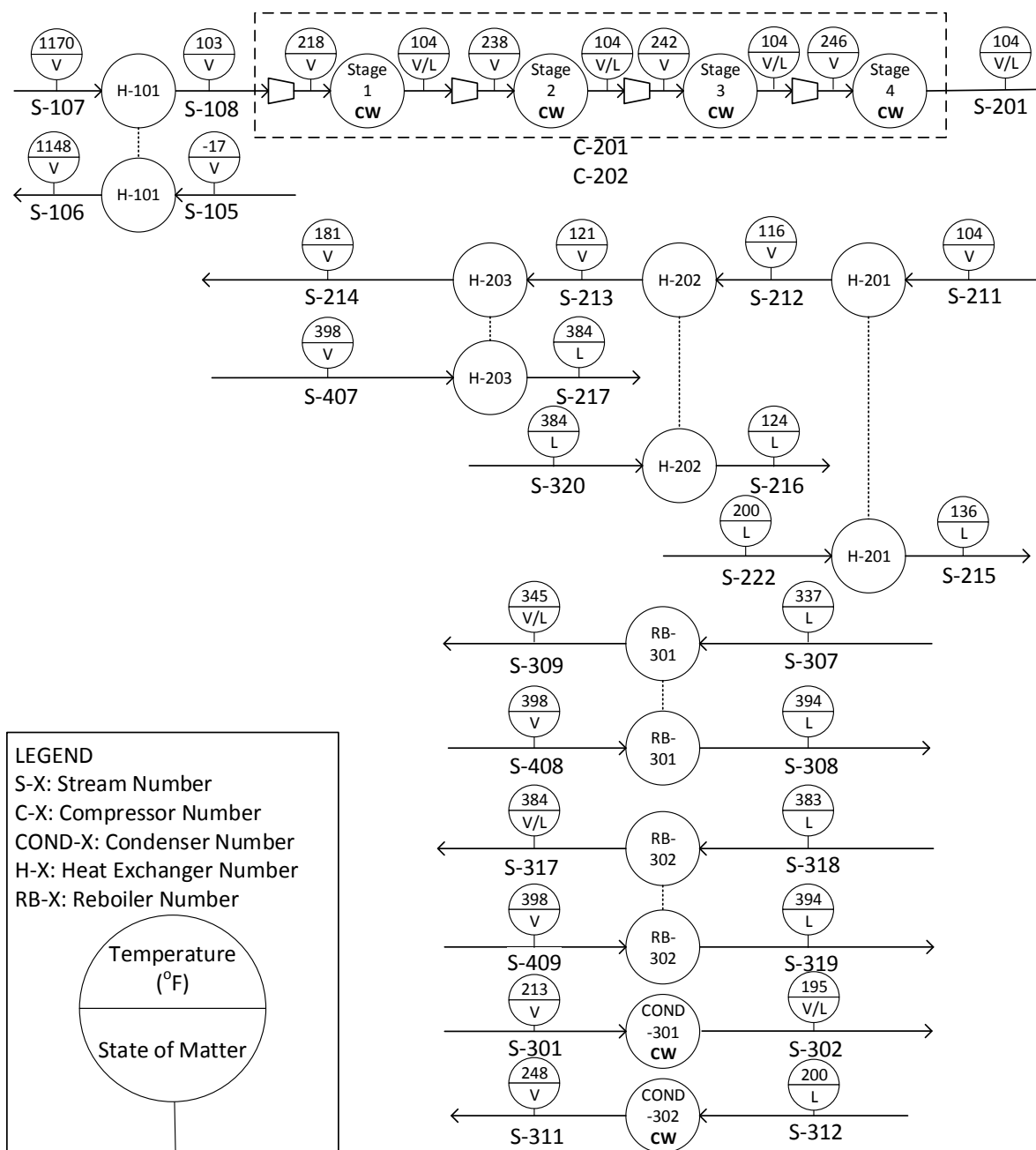


Figure 12. Heat Exchanger Network for the Process.

Tables 19-30. Heat Exchanger Network Tables.

Unit	H-101			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°F)	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 (°F)
Cold out	S-106	1148	53340	57.8

Unit	C-101 Stage 1			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°F)	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 (°F)
Cold out	CW	120	7166	43.2

Unit	C-101 Stage 2			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°F)	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 (°F)
Cold out	CW	120	6342	48.8

Unit	C-101 Stage 3			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°F)	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 (°F)
Cold out	CW	120	5996	49.9

Unit	C-101 Stage 4			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°F)	Heat duty (MMBTU/hr)
Hot in	S-108	246	149.7	44.07
Hot out	S-108	140		
Cold in	CW	90	Area (ft ²)	LMTD (°F)
Cold out	CW	120	3580	82.2

Unit	H-201			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (ft ²)	LMTD (°F)
Cold out	S-212	115	433.6	53.9

Unit	H-202			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (ft ²)	LMTD (°F)
Cold out	S-213	120	133.0	73.0

Unit	H-203			
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (ft ²)	LMTD (°F)
Cold out	S-214	181	478.5	239

Unit		RB-301		
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (°F)
Cold out	S-309	349	2371	55.0

Unit		RB-302		
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (°F)
Cold out	S-318	387	13260	12.4

Unit		COND-301		
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (°F)
Cold out	CW	120	150	98.9

Unit		COND-302		
	Stream	Temperature (°F)	U (Btu/hr-ft ² -°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 (°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°F to 104°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°F to 186°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 ft². The shell-side pressure is kept at 83 psig. COND-301 has an overall heat transfer coefficient of 250 Btu/hr-ft²-°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°F to 196°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 ft². The shell-side pressure is kept at 2.3 psig. COND-302 has an overall heat transfer coefficient of 250 Btu/hr-ft²-°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°F to 1350°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°F to 116°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°F to 136°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 ft². The shell-side pressure will be kept at 705.3 psig. H-201 has an overall heat transfer coefficient of 149.7 Btu/hr-ft²-°F 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° F to 121° 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°F to 124°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 ft². The shell-side pressure will be kept at 695.3 psig. H-202 has an overall heat transfer coefficient of 149.7 Btu/hr-ft²-°F 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°F to 181°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° F to 384° 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 ft². The shell-side pressure will be kept at 685.3 psig. H-203 has an overall heat transfer coefficient of 149.7 Btu/hr-ft²-°F 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°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°F and 43.7 psia. The outlet from the reactor, S-107, has a mass flow rate of 570,023 lb/hr at 1166°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°F to 394°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 ft². The shell-side pressure is kept at 84.3 psig. RB-301 has an overall heat transfer coefficient of 250 Btu/hr-ft²-°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°F to 394°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 ft². The shell-side pressure is kept at 16.3 psig. RB-301 has an overall heat transfer coefficient of 250 Btu/hr-ft²-°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°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 °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°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°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° F to -27° 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° F to -37° 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° F to 165° 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° F to 398° 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					
Materials Handled	Mass Flow (lb/hr)				
	Feed	Exit 1	Exit 2	Exit 3	Exit 4
	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 Principles¹⁴			

Condensers

CONDENSER		
Identification: COND-301		
Function: Partially condenses the vapor from the top of COL-301 from 213°F to 195°F		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

CONDENSER		
Identification: COND-302		
Function: Condenses the vapor from the top of COL-302 from 248°F to 200°F		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

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			
Materials Handled:	Mass Flow (lb/hr)		
	Feed	Exit 1	Exit 2
	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 Principles¹⁴		

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					
Materials Handled:	Mass Flow (lb/hr)				
	Feed 1	Feed 2 (Reflux)	Feed 3 (Boil up)	Exit 1	Exit 2
	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 Principles¹⁴				

DISTILLATION COLUMN					
Identification: COL-302					
Function: Takes the bottoms product of COL-301 and separates BTX compounds from heavier hydrocarbons.					
Operation: Continuous					
Materials Handled:	Mass Flow (lb/hr)				
	Feed	Feed (Reflux)	Feed (Boil up)	Exit 1 (Distillate)	Exit 2 (Bottoms)
	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 Principles¹⁴				

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					
Materials Handled:	Mass Flow (lb/hr)				
	Combustion Side			Water Side	
	Feed 1	Feed 2	Exit 1	Feed 3	Exit 2
	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				
Materials Handled:	Mass Flow (lb/hr)			
	Feed 1 (Hot)	Exit 1 (Hot)	Feed 2 (Cold)	Exit 2 (Cold)
	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				
Materials Handled:	Mass Flow (lb/hr)			
	Feed 1 (Hot)	Exit 1 (Hot)	Feed 2 (Cold)	Exit 2 (Cold)
	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 Principles¹⁴			

HEAT EXCHANGER				
Identification: H-202				
Function: Exchange heat between H-201's shell side stream and COL 302's liquid product.				
Operation: Continuous				
Materials Handled:	Mass Flow (lb/hr)			
	Feed 1 (Hot)	Exit 1 (Hot)	Feed 2 (Cold)	Exit 2 (Cold)
	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 Principles¹⁴			

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				
Materials Handled:	Mass Flow (lb/hr)			
	Feed 1 (Hot)	Exit 1 (Hot)	Feed 2 (Cold)	Exit 2 (Cold)
	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 Principles¹⁴			

Pressure Vessel

PRESSURE VESSEL	
Identification: PV-101	
Function: Stores a regeneration cycle's worth of chlorine.	
Operation: Batch	
Materials Handled:	Mass Flow (lb/hr)
	Exit
	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 Principles¹⁴

PRISM Unit

PRISM			
Identification: PR-201			
Function: Separates hydrogen and methane from its feed stream, S-214, using membrane separation.			
Operation: Continuous			
Materials Handled:	Mass Flow (lb/hr)		
	Feed	Exit 1	Exit 2
	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		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

PUMP		
Identification: P-301		
Function: Pumps the liquid reflux from the reflux accumulator RA-301 to the distillation column, COL-301.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

PUMP		
Identification: P-302		
Function: Pumps the liquid from the bottom of the column COL-301 to the reboiler RB-301.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

PUMP		
Identification: P-303		
Function: Pumps the liquid reflux from the reflux accumulator RA-302 to the distillation column, COL-302.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

PUMP		
Identification: P-304		
Function: Pumps the liquid from the bottom of the column COL-302 to the reboiler RB-302.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

PUMP		
Identification: P-401		
Function: Pumps water to the steam boiler.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

Reactor

REACTOR		
Identification: R-101, R-102, R-103		
Function: Converts ethane feedstock to desired BTX product.		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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					
Materials Handled:	Mass Flow (lb/hr)				
	Hot Side		Cold Side		
	Feed 1	Exit 1	Feed 2	Exit 2	Exit 3
	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 Principles¹⁴				

REBOILER					
Identification: RB-302					
Function: Uses high pressure steam to vaporize the liquid leaving the bottom of distillation column COL-302.					
Operation: Continuous					
Materials Handled:	Mass Flow (lb/hr)				
	Hot Side		Cold Side		
	Feed 1	Exit 1	Feed 2	Exit 2	Exit 3
	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 Principles¹⁴				

Reflux Accumulators

REFLUX ACCUMULATOR			
Identification: RA-301			
Function: Stores reflux from top of column to maintain constant reflux and distillate flow rates.			
Operation: Continuous			
Materials Handled:	Mass Flow (lb/hr)		
	Feed	Exit 1	Exit 2
	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 Principles¹⁴		

REFLUX ACCUMULATOR			
Identification: RA-302			
Function: Stores reflux from top of column to maintain constant reflux and distillate flow rates.			
Operation: Continuous			
Materials Handled:	Mass Flow (lb/hr)		
	Feed	Exit 1	Exit 2
	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 Principles¹⁴		

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	
Materials Handled:	Mass Flow (lb/hr)
	Feed
	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 Principles¹⁴

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	
Materials Handled:	Mass Flow (lb/hr)
	Feed
	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 Principles¹⁴

Turbines

TURBINE		
Identification: T-101, T-102, T-103		
Function: To recover work from permeate coming out of PRISM		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

TURBINE		
Identification: T-104		
Function: To recover work from feedstock ethane		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

TURBINE		
Identification: T-105		
Function: To recover work from distillate from the first distillation column's reflux accumulator		
Operation: Continuous		
Materials Handled:	Mass Flow (lb/hr)	
	Feed	Exit
	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 Principles¹⁴	

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				
Materials Handled:	Mass Flow (lb/hr)			
	Feed	Exit 1	Exit 2	Exit 3
	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 Principles¹⁴			

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

Equipment Cost Summary

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.

<u>Operations</u>	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
<u>Maintenance</u>	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
<u>Operating Overhead</u>	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
<u>Property Taxes and Insurance</u>	Annual Cost

Property Taxes and Insurance:	\$6,066,358
<u>Total Fixed Costs</u>	\$43,408,526

Guidelines provided in Chapter 23 of Product and Process Design Principles¹⁴ 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.

<u>Variable Costs at 100% Capacity:</u>			
<u>General Expenses</u>			
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
<u>Raw Materials</u>	\$0.341	per lb of BTX	\$318,535,578
<u>Byproducts</u>	\$0.113	per lb of BTX	(\$102,397,305)
<u>Utilities</u>	\$0.030	per lb of BTX	\$27,762,245
<u>Total Variable Costs</u>			\$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 Principles¹⁴. 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

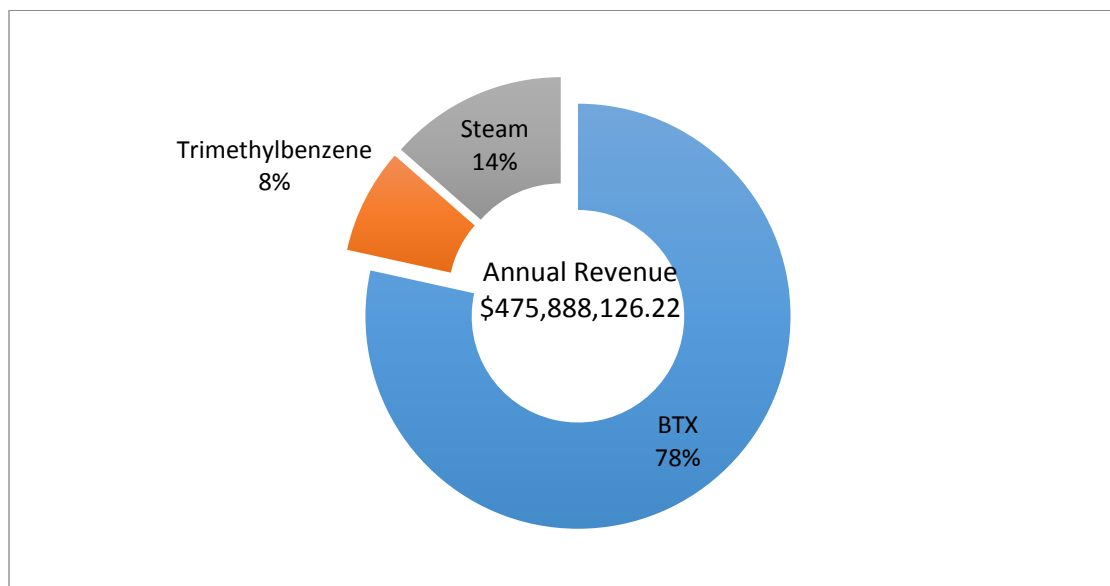


Figure 10. Revenue Stream Analysis

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

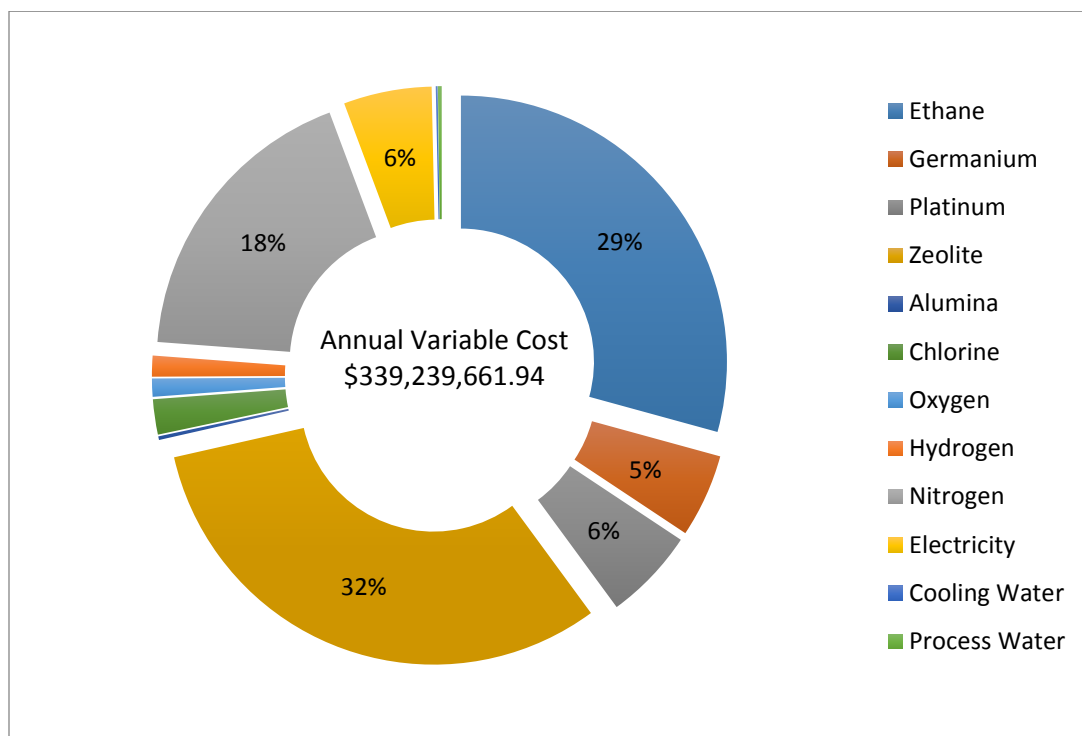


Figure 11. Variable Cost Analysis

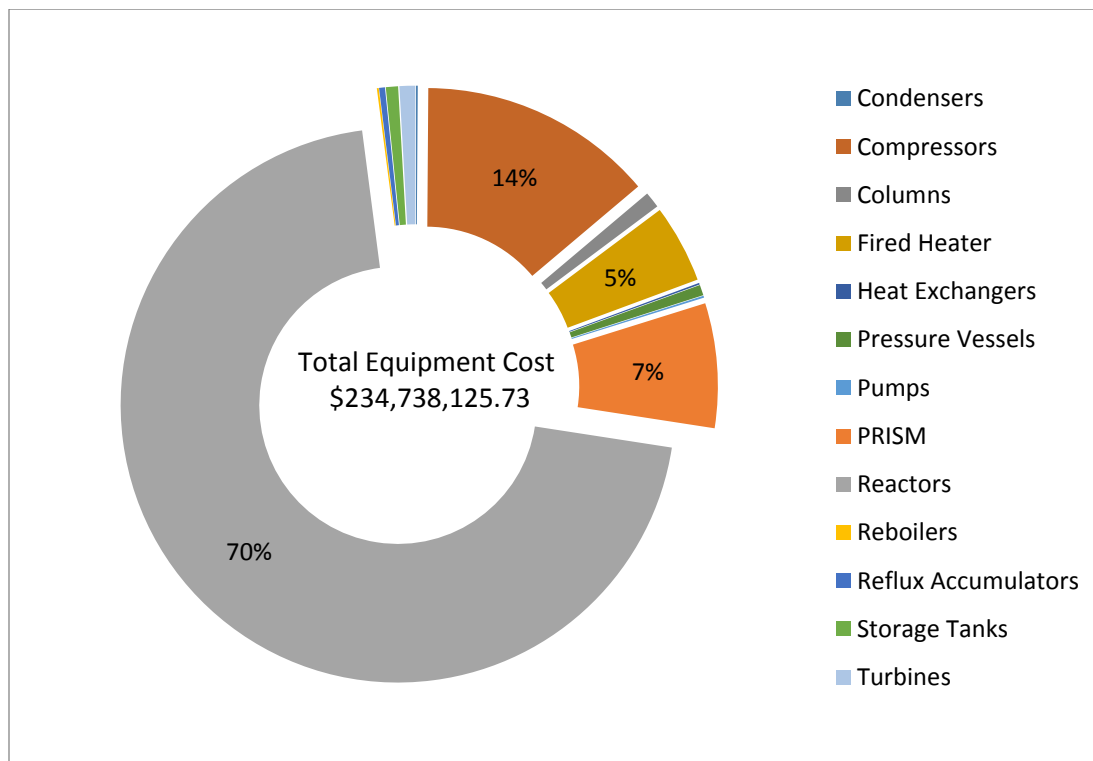


Figure 12. Equipment Cost Analysis

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

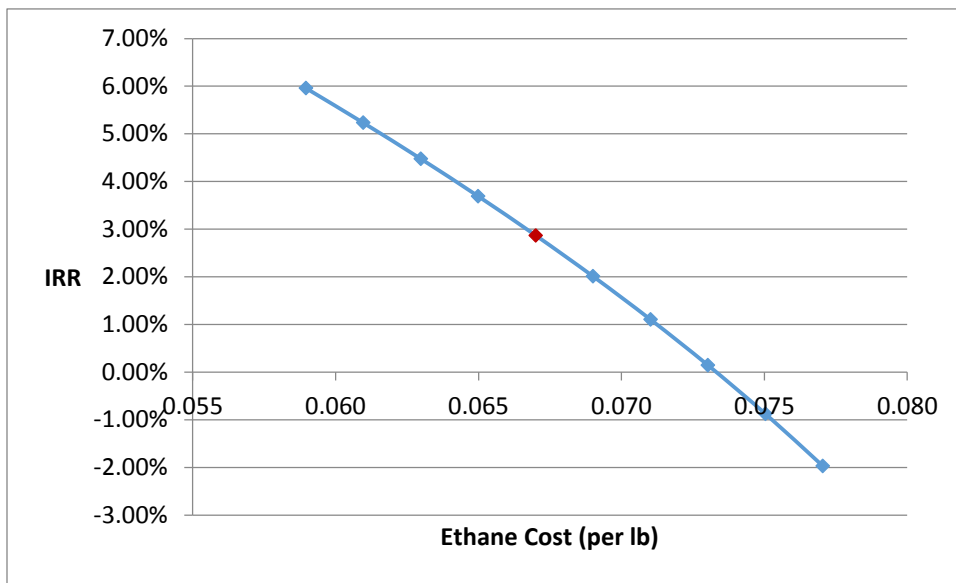


Figure 13. Effect of Ethane Price on IRR

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

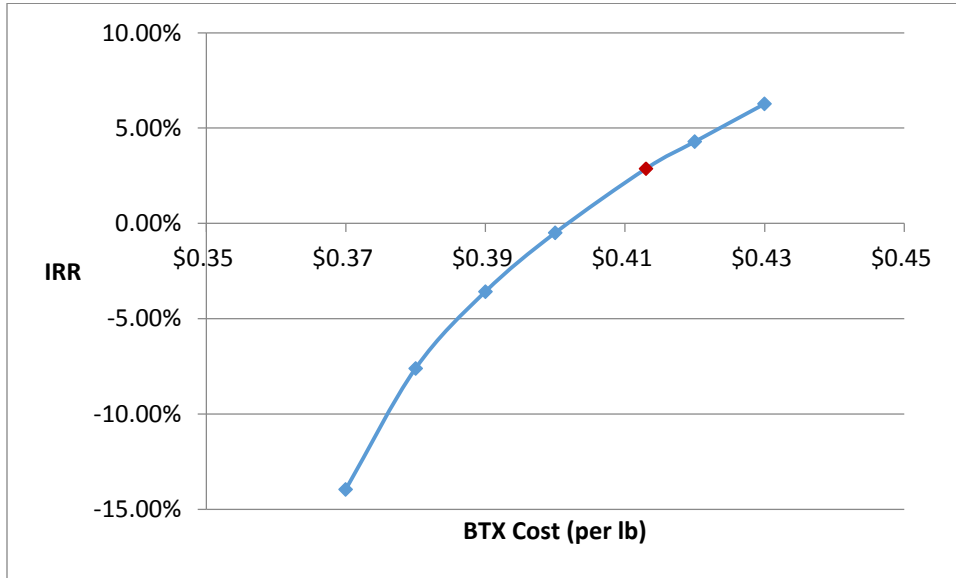


Figure 14. Effect of BTX price on IRR

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.

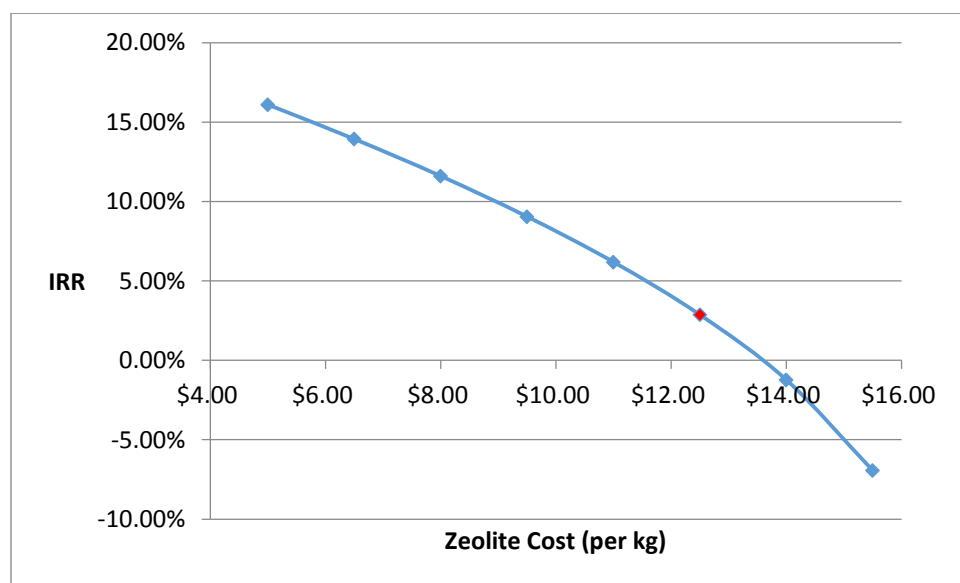
Sensitivity Analysis on Catalyst Cost

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

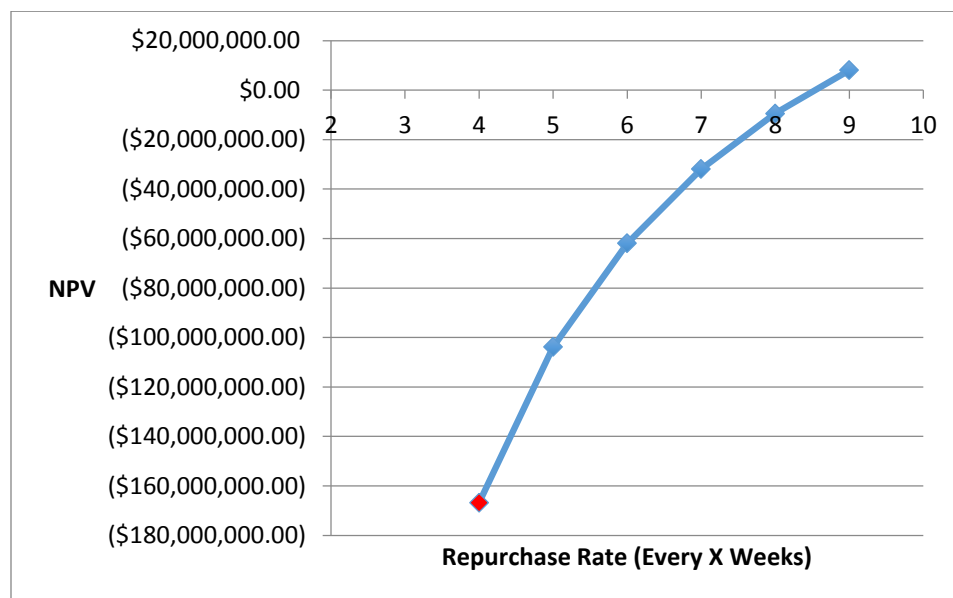


Figure 16. Effect of catalyst lifetime on NPV

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 chosen²⁵.

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 columns²³ and flash vessels are associated with failure modes such as overheating, impurities, and leaks⁶. 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 process⁸. 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 cost¹³. 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 CO₂ 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 steel²⁴; 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 plants⁸.

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-ft²-°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:

$$T_{\text{hot,in}} = 200.2^{\circ}\text{F}$$

$$T_{\text{hot,out}} = 136.4^{\circ}\text{F}$$

$$T_{\text{cold,in}} = 104.0^{\circ}\text{F}$$

$$T_{\text{cold,out}} = 116.1^{\circ}\text{F}$$

$$Q = 3497690 \text{ BTU/hr}$$

Calculation of Log Mean Temperature Difference:

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

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

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

Calculation of area:

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

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*10⁶ ft³/h. Reactor volume was then calculated as follows:

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

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:

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

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 al¹³.

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}	Height of the head Space
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
ρ_L	Density of the liquid
ρ_V	Density of the vapor
σ	Surface Tension

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

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

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

$$H = 77 \text{ ft}$$

Assuming

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

U_f may be calculated by using equation 3.

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

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.

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

σ 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.

σ 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 σ 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/ft³ and 0.932 lb/ft³ 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 surface
n_{O_2}	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.

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

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.



The number of moles of oxygen, n_{O_2} , 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 guidelines 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					
<u>Year</u>	<u>Action</u>	<u>Distribution of Permanent Investment</u>	<u>Production Capacity</u>	<u>Depreciation</u> 5 year MACRS	<u>Product Price</u>
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		
<u>Equipment Description</u>		<u>Bare Module Cost</u>
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

Appendix A-3. Profitability Analysis Spreadsheet

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 BTX	\$0.18 per lb

Appendix A-3. Profitability Analysis Spreadsheet

BTX

Total Weighted Average:	\$0.353 per lb of BTX
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Byproducts

<u>Byproduct:</u>	<u>Unit:</u>	<u>Ratio to Product</u>	<u>Byproduct Selling Price</u>
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
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Utilities

<u>Utility:</u>	<u>Unit:</u>	<u>Required Ratio</u>	<u>Utility Cost</u>
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				
<u>General Expenses:</u>				
		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				
<u>Operations</u>				
		Operators per Shift:	8	(assuming 5 shifts)
		Direct Wages and Benefits:	\$40	/operator hour

Appendix A-3. Profitability Analysis Spreadsheet

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
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Straight Line Depreciation

Direct Plant:	8.00%	of Total Depreciable Capital, less 1.18 times the Allocated Costs
Allocated Plant:	6.00%	for Utility Plants and Related Facilities
		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
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<u>Raw Materials</u>	\$0.352842	per lb of BTX	\$318,535,578
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<u>Byproducts</u>	\$0.113426	per lb of BTX	(\$102,397,305)
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<u>Utilities</u>	\$0.030752	per lb of BTX	\$27,762,245
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<u>Total Variable Costs</u>	\$	287,013,885
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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
<u>Property Taxes and Insurance</u>		
Property Taxes and Insurance:	\$	6,066,358
<u>Other Annual Expenses</u>		
Rental Fees (Office and Laboratory Space):	\$	-
Licensing	\$	-
Fees:	\$	-
Miscellaneous:	\$	-
Total Other Annual Expenses	\$	-
<u>Total Fixed Costs</u>	\$	<u>43,408,526</u>

Investment Summary

Total Bare Module Costs:

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

Appendix A-3. Profitability Analysis Spreadsheet

	\$	1,474,758
Other Equipment	\$	-
Catalysts	\$	-
Computers, Software, Etc.	\$	-
<u>Total Bare Module Costs:</u>	\$	<u>233,680,967</u>

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:	\$	-
<u>Direct Permanent Investment</u>	\$	<u>257,049,064</u>

Total Depreciable Capital

Cost of Contingencies & Contractor Fees	\$	46,268,832
<u>Total Depreciable Capital</u>	\$	<u>303,317,896</u>

Total Permanent Investment

Cost of Land:	\$	6,066,358
Cost of Royalties:	\$	-
Cost of Plant Start-Up:	\$	30,331,790
Total Permanent Investment - Unadjusted		

Appendix A-3. Profitability Analysis Spreadsheet

Site Factor	\$ 339,716,043
	1.00
<u>Total Permanent Investment</u>	<u>\$ 339,716,043</u>

Working Capital

	<u>2016</u>	<u>2017</u>	<u>2018</u>
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
<i>Present Value at 18%</i>	\$ 4,912,036	\$ 1,387,581	\$ 1,175,916

<u>Total Capital Investment</u>	<u>\$ 347,191,577</u>
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A-3.3. Cash Flows

Cash Flow Summary

<u>Year</u>	<u>Percentage of Design Capacity</u>	<u>Product Unit Price</u>	<u>Sales</u>	<u>Capital Costs</u>	<u>Working Capital</u>	<u>Var Costs</u>	<u>Fixed Costs</u>	<u>Depreciation</u>	<u>Depletion Allowance</u>	<u>Taxable Income</u>
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)	-	(65,200)
2018	60%	\$0.42	227,325,000	-	(1,932,100)	(174,791,500)	(44,059,700)	(97,061,700)	-	(88,500)
2019	75%	\$0.43	288,418,600	-	(1,932,100)	(221,766,700)	(44,720,500)	(58,237,000)	-	(36,300)
2020	90%	\$0.43	351,293,900	-	-	(270,111,800)	(45,391,400)	(34,942,200)	-	848,500
2021	90%	\$0.44	356,563,300	-	-	(274,163,500)	(46,072,200)	(34,942,200)	-	1,385,000
2022	90%	\$0.45	361,911,700	-	-	(278,275,900)	(46,763,300)	(17,471,100)	-	19,400
2023	90%	\$0.45	367,340,400	-	-	(282,450,100)	(47,464,800)	-	-	37,420
2024	90%	\$0.46	372,850,500	-	-	(286,686,800)	(48,176,700)	-	-	37,980
2025	90%	\$0.47	378,443,300	-	-	(290,987,100)	(48,899,400)	-	-	38,550
2026	90%	\$0.47	384,119,900	-	-	(295,351,900)	(49,632,900)	-	-	39,130
2027	90%	\$0.48	389,881,700	-	-	(299,782,200)	(50,377,400)	-	-	39,720
2028	90%	\$0.49	395,730,000	-	-	(304,278,900)	(51,133,000)	-	-	40,310
2029	90%	\$0.49	401,665,900	-	-	(308,843,100)	(51,900,000)	-	-	40,920
2030	90%	\$0.50	407,690,900	-	-	(313,475,800)	(52,678,500)	-	-	41,530
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	<u>(3,304,894)</u>	
Total Capital Investment		<u>351,308,449</u>
ROI	-0.94%	

Sensitivity Analyses

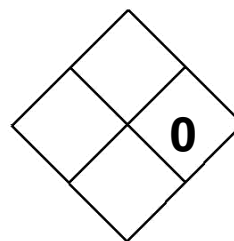
Note: The Sensitivity Analyses section below takes quite a bit of memory to update each time a cell is changed; therefore, automatic calculations are turned off. After making your axis selections, print the IRR values. (These two lines may be deleted before printing.)

Appendix A-3. Profitability Analysis Spreadsheet

		Vary Initial Value by +/-									
x-axis		15%									
y-axis		15%									
Product Price						Variable Costs					
		\$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



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.**Contact Information:****Sciencelab.com, Inc.**14025 Smith Rd.
Houston, Texas 77396US 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**Synonym:** Benzol; Benzine**Chemical Name:** Benzene**Chemical Formula:** C₆-H₆

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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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, CO₂).

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 powerful 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. Vigorous 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 nitril 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 powerful 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, dimanganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powerful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonosulfuric 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:

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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

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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

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MATERIAL SAFETY DATA SHEET

SECTION 1. PRODUCT

IDENTIFICATION PRODUCT NAME: Carbon Dioxide

CHEMICAL NAME: Carbon Dioxide **FORMULA:** CO₂

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:

Not Applicable
Nonflammable

AUTOIGNITION:

Nonflammable

FLAMMABLE LIMITS:

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/ft³ (1.832 kg/m³)

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

SPECIFIC GRAVITY (Air =1): 1.522

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

BOILING POINT: -109.3 F (-78.5 C)

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

SOLUBILITY IN WATER (Vol./Vol. at 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:

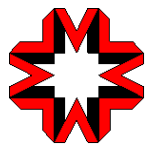
CALIFORNIA:

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:	
HEALTH:	1		HEALTH:	0
FLAMMABILITY:	0		FLAMMABILITY:	0
REACTIVIT	0		REACTIVITY:	0
Y: 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 3 rd Floor Philamlife, 126 L.P. Leviste St. Salcedo Village, Makati City For Assistance Call : (02) 817-8971 to 76 loc 214; Direct line (02) 817-1830
Iligan Plant	Assumption Heights, Iligan City Tel: (063) 221-9466, 221-1190
Mabuhay Premium Bleach Plant	LTAL, Brgy. Biñan, Biñan, Laguna Tel: (049) 541-1923
Batangas Depot	BBTI Compound, Bauan, Batangas Tel: (043) 980-5869
Cebu Depot	Ceniza St., Ouan, Mandaue City Tel: (032) 344-5259, 345-0639
Davao Depot	Bunawan, Davao City 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

V. FIRE FIGHTING MEASURES

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.

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.



Safety Data Sheet CHLORINE

Appendix A-4. MSDS Information

MVC-MSDS-C-
001P Issue Date :
11/15/13 Rev. Code
: 03

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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 1 ppm STEL
Europe	0.5 ppm STEL; 1.5 mg/m ³ STEL
OSHA (Final)	1 ppm Ceiling; 3 mg/m ³ Ceiling
OSHA (Vacated)	0.5 ppm TWA; 1.5 mg/m ³ TWA

NIOSH

1 ppm STEL; 3 mg/m³ STEL

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.

Appendix A-4. MSDS Information

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:

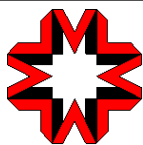
- Any air-purifying, full-facepiece respirator (gas mask) with a chin-style, front- or back-mounted canister providing protection against the compound of concern

- 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

Appendix A-4. MSDS Information

MVC-MSDS-C-
001P Issue Date :
11/15/13 Rev. Code
: 03

Page 5 of 5

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.

Environmental Hazards

Marine Pollutant : Yes

Environmentally Hazardous : Yes
No

IMDG

ADR/RID

IATA

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

UN Proper Shipping Name

Transport hazard class

Packing group

1017

CHLORINE

2.3(Toxic Gas, Corrosive,
Oxidizing)

Not applicable



Label

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
Revision date : 04.01.2011

Version : 2.0

DE / E

SDS No. : 051a
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 leak can 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 coordination. 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
Revision date : 04.01.2011

Version : 2.0

DE / E

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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
Revision date : 04.01.2011

Version : 6.0

DE / E

SDS No. : 055a
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 advice/attention.

P377

Leaking gas fire: Do not extinguish, unless leak can 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 coordination. 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
Revision date : 04.01.2011

Version : 6.0

DE / E

SDS No. : 055a
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



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/ft ³ (70.96 kg/m ³)
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) @ 70°F (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 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
Trade Name: **CBV2314**
 I N T E R N A T I O N A L

ZEOLITE AMMONIUM ZSM-5 POWDER

Date

Prepared: **03/14/06**

Page: **1 of 4**

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

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

2. COMPOSITION/INFORMATION ON

INGREDIENTS

<i>Chemical and Common</i>	<i>CAS Registry</i>	<i>Wt. %</i>	<i>OSHA PEL</i>	<i>ACGIH TLV</i>
<i>Name</i>	<i>Number</i>			
Zeolite	1318-02-1	100%	15mg/m³ total dust	10 mg/m³
			5mg/m³ respirable	3 mg/m³ respirable

3. HAZARDS IDENTIFICATION

<i>Emergency Overview:</i>	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.
<i>Eye contact:</i>	Causes mild eye irritation.
<i>Skin contact:</i>	Prolonged or repeated contact may dry skin and cause irritation.
<i>Inhalation:</i>	Causes irritation.
<i>Ingestion:</i>	No known hazards. Inedible.
<i>Chronic hazards:</i>	No known hazards.
<i>Physical hazards:</i>	Absorbs water from air and fluids. Generates heat when it absorbs water.

4. FIRST AID MEASURES

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

Trade Name: **CBV2314**

ZEOLITE AMMONIUM ZSM5 POWDER

Date

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*Page:***2 of 4**

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

reuse.

Remove to fresh air. If not breathing, give artificial respiration. If breathing

Inhalation:

is difficult, give oxygen. Get medical attention.

Ingestion:

Not applicable.

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 known 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.

7. HANDLING AND STORAGE

Avoid contact with eyes, skin and clothing. Avoid breathing dust.

Handling:

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**

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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.**



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, 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:

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 ACGIH Consult 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 Santé et de la Sécurité du Travail du Québec. -SAX, N.I. Dangerous Properties of Industrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du règlement sur le transport des marchandises dangereuses au Canada. Centre de conformité internationale Ltée. 1986.

Other Special Considerations: Not available.

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

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Manufactured for

**INDUSTRIAL SCIENTIFIC
CORPORATION**1001 Oakdale Road
Oakdale, PA 15071-1500Phone (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:** CH₄**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 Cambridge, MD 21613
EMERGENCY PHONE:	CHEMTREC: 1-800-424-9300
BUSINESS PHONE:	1-410-228-6400
	1-713/868-0440
	1-800/231-1366
	General MSDS Information:
	Fax on Demand:

2. COMPOSITION and INFORMATION ON INGREDIENTS

CHEMICAL NAME	CAS #	mole %	EXPOSURE LIMITS IN AIR					
			ACGIH-TLV		OSHA-TLV		NIOSH IDLH	OTHER
			TWA ppm	STEL ppm	TWA ppm	STEL 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%

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.

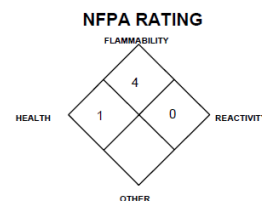
UNUSUAL FIRE AND EXPLOSION HAZARDS: When involved in a fire, this material may decompose and produce toxic gases including carbon monoxide and carbon dioxide.

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/ft³
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 (ft³/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 2.1 (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/NDL 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**

This Material Safety Data Sheet is offered pursuant to OSHA's Hazard Communication Standard, 29 CFR, 1910.1200. Other government regulations must be reviewed for applicability to this product. To the best of CALGAZ knowledge, the information contained herein is reliable and accurate as of this date; however, accuracy, suitability or completeness are not guaranteed and no warranties of any type, either express or implied, are provided. The information contained herein relates only to this specific product. If this product is combined with other materials, all component properties must be considered. Data may be changed from time to time. Be sure to consult the latest edition.



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) Nitrogen, Instrument Grade Nitrogen, Pharmaceutical Grade 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, 3/4 inch BSP right hand female valves.
Company Identification	African Oxygen Limited 23 Webber Street Johannesburg, 2001 Tel No: (011) 490-0400 Fax No: (011) 490-0506 0860 020202 or (011) 873 4382 (24 hours)
EMERGENCY NUMBER	

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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The Stripe Symbol and the word "AFROX" are AFROX Group Trademarks.

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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 away 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:** O₂
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:

Not applicable

AUTOIGNITION:

Nonflammable

FLAMMABLE LIMITS:

Nonflammable

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

HAZARDOUS COMBUSTION PRODUCTS: None

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

UNUSUAL FIRE AND EXPLOSION HAZARDS: Oxygen vigorously accelerates combustion. Some materials which are noncombustible in air will burn in the presence of an oxygen enriched atmosphere (greater than 23%). Fire resistant clothing may burn and offer no protection in oxygen rich atmospheres. Oxygen may form explosive compounds when exposed to combustible materials or oil, grease, and other hydrocarbon materials. Pressure in a

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

SECTION 6. ACCIDENTAL RELEASE MEASURES

Evacuate all personnel from affected area. Shut off source of oxygen if possible. Increase ventilation to release area. Personnel who have been exposed to high concentrations of oxygen should stay in a well-ventilated or open area for 30 minutes before going into a confined space or near an ignition source.

If leak is from container or its valve, call the Air Products emergency telephone number. If leak is in user's system close cylinder valve and vent pressure before attempting repairs.

SECTION 7. STORAGE AND HANDLING

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

HANDLING: Do not drag, roll, or slide cylinder. Use a suitable handtruck designed for cylinder movement. Never attempt to lift a cylinder by its cap. Secure cylinders at all times while in use. Use a pressure reducing regulator or separate control valve to safely discharge gas from cylinder. Use a check valve to prevent reverse flow into cylinder. Do not 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.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE: Colorless gas

ODOR: Odorless

MOLECULAR WEIGHT: 32.0

BOILING POINT (1 atm): -297.3 °F (-183.0 °C)

SPECIFIC GRAVITY (Air =1): 1.10

SPECIFIC VOLUME (at 70 °F 21.1 °C) and 1 atm): 12.08 ft³/lb (0.754 m³/kg)

FREEZING / MELTING POINT: -361.9 °F (-218.8 °C)

VAPOR PRESSURE: Not applicable at 70°F

GAS DENSITY (At 70°F (21.1°C) and 1 Atm): 0.083 lb /ft³ (1.326 kg/m³)

SOLUBILITY IN WATER (Vol./Vol. at 32°F (0°C)): 0.049

SECTION 10. REACTIVITY / STABILITY

CHEMICAL STABILITY: Stable

CONDITIONS TO AVOID: None

INCOMPATIBILITY: Oils, grease, hydrocarbons and flammable materials.

HAZARDOUS DECOMPOSITION PRODUCTS: None

HAZARDOUS POLYMERIZATION: Will not occur

SECTION 11. TOXICOLOGICAL INFORMATION

At atmospheric concentration and pressure, oxygen poses no toxicity hazards.

Premature infants exposed to high oxygen concentrations may suffer delayed retinal damage which can progress to retinal detachment and blindness. Retinal damage may also occur in adults exposed to 100% oxygen for extended periods (24 to 48 hr).

At two or more atmospheres central nervous system (CNS) toxicity occurs. Symptoms include nausea, vomiting, dizziness or vertigo, muscle twitching, vision changes, and loss

of consciousness and generalized seizures. At three atmospheres, CNS toxicity occurs in less than two hours, and at six atmospheres in only a few minutes.

SECTION 12. ECOLOGICAL INFORMATION

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

SECTION 13. DISPOSAL

UNUSED PRODUCT / EMPTY CONTAINER: Return container and unused product to supplier. Do not attempt to dispose of residual or unused quantities.

DISPOSAL: For emergency disposal, secure cylinder and slowly discharge gas to the atmosphere in a well ventilated area or outdoors.

SECTION 14. TRANSPORTATION

DOT HAZARD CLASS: 2.2 (Nonflammable Gas) **DOT SHIPPING LABEL:** Nonflammable Gas,

Oxidizer

DOT SHIPPING NAME: Oxygen, compressed

IDENTIFICATION NUMBER: UN 1072

REPORTABLE QUANTITY (RQ): None

PLACARD: Nonflammable Gas or Oxygen

SPECIAL SHIPPING INFORMATION: Cylinders should be transported in a secure upright position in a well ventilated truck. Never transport in passenger compartment of a vehicle. An oxygen label may be used for domestic shipment in the United States and Canada in place of the Non-flammable and Oxidizer labels (49CFR Part 172).

SECTION 15. REGULATORY INFORMATION

U.S. FEDERAL REGULATIONS:

EPA - ENVIRONMENTAL PROTECTION AGENCY:

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

CERCLA Reportable Quantity: None

SARA TITLE III: Superfund Amendments and Reauthorization Act of 1986

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

Oxygen is not listed as an Extremely Hazardous Substance.

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



IMMEDIATE: No
DELAYED: No
PRESSURE: s
REACTIVITY: No
FIRE: s

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**

Sheet

o-Xylene MSDS

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Section 1: Chemical Product and Company Identification

Product Name: o-Xylene**Catalog Codes:** SLX1012**CAS#:** 95-47-6**RTECS:** ZE2450000**Contact Information:****Sciencelab.com, Inc.**14025 Smith Rd.
Houston, Texas 77396US Sales: **1-800-901-7247**International Sales: **1-281-441-4400****TSCA:** TSCA 8(b) inventory: o-XyleneOrder Online: ScienceLab.com**CI#:** Not applicable.**CHEMTREC (24HR Emergency Telephone), call:**

1-800-424-9300

International CHEMTREC, call: 1-703-527-3887**Synonym:** 1,2-Dimethylbenzene**Chemical Name:** o-Xylene**For non-emergency assistance, call:** 1-281-441-4400**Chemical Formula:** C₆H₄(CH₃)₂

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, 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. 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
<p>Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.</p> <p>Large Spill:</p>

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 NIOSH Consult 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)
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Volatility: Not available.

Odor Threshold: 0.05 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; $\log(\text{oil/water}) = 3.1$

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 Effects 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 Santé et de la Sécurité du Travail du Québec. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du règlement sur le transport des marchandises dangereuses au Canada. Centre de conformité international Ltée. 1986.

Other Special Considerations: Not available.**Created:** 10/11/2005 12:54 PM**Last Updated:** 05/21/2013 12:00 PM

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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:** C₃H₈**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

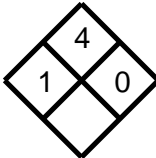
INGREDIENT NAME /CAS NUMBER	PERCENTAGE	OSHA PEL	ACGIH	TLV
Propane / 74-98-6	87.5 -100		Simple asphyxiant	
Ethane / 74-84-0	0 - 7.0		Simple asphyxiant	
Propylene / 115-07-1	0 - 5.0	1,000 ppm	Simple asphyxiant	
Butanes / 106-97-8	0 - 2.5		Simple asphyxiant	
Ethyl Mercaptan / 75-08-1.....	0 - 50 ppm		0.5 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.

	FIRE HAZARD (Red)	
HEALTH HAZARD (Blue)		REACTIVITY (Yellow)
	SPECIAL	HAZARDS*
Minimal 0	Moderate 2	Severe 4
Slight 1	Serious 3	*(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.

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, CO₂, 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 ₃ H ₆ or CH ₃ CH: CH ₂

PHYSICAL DATA

▪MOLECULAR WEIGHT	42.081
▪FREEZING POINT	
▪BOILING POINT	-185.2°C, -301.4°F
▪VAPOR PRESSURE	-47.7°C, -53.9 °F
▪SPECIFIC VOLUME	942 kPa (gauge), 136.5 psig
▪RELATIVE DENSITY, (air=1)	0.567 m ³ /kg, 9.06ft ³ /lb @ 1 atm, 21.1°C
▪SOLUBILITY IN WATER	1.48 @ 1 atm, 20°C
▪DESCRIPTION	22.05 cm ³ /100 ml @ 1 atm, 20°C

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	
▪ UNUSUAL HAZARDS	

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.

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
- ACCUTE EFFECTS OVEREXPOSURE
- CHRONIC EFFECTS OF OVEREXPOSURE

OSHA TWA None established.

ASGIH TWA None established.

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.

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
- INCOMPATIBILITY
- HAZARDOUS DECOMPOSITION/

(X) Stable. () Unstable.

Oxidizing material.

Carbon monoxide, carbon dioxide

OXIDATION PRODUCTS

- 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.
2. Respiratory protection – Approved respiratory equipment must be worn when airborne concentrations exceed safe levels.
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.
2. Install check valves or traps to prevent suckback to the cylinder.
3. Ground all lines and equipment.
4. Leak check the lines and equipment.

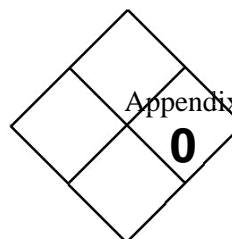
5. Have an emergency plan covering steps to be taken in the event of an accidental release.

DISCLAIMER

The information, recommendations, and suggestions herein were compiled from reference material and other sources believed to be reliable. However, the MSDS's accuracy or completeness is not

guaranteed by Gas Innovations or its affiliates, nor is any responsibility assumed or implied for any loss or damage resulting

from inaccuracies or omissions. Since conditions of use are beyond our control, no warranties of merchantability of fitness for a particular purpose are expressed or implied. This MSDS is not intended as a license to operate under, or recommendation to infringe on, any patents. Appropriate warnings and safe handling procedures should be provided to handlers and users



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.

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

Synonym: p-Methyltoluene

Chemical Name: 1,4-Dimethylbenzene

Chemical Formula: C₆H₄(CH₃)₂

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
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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 ACGIH Consult 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 Santé et de la Sécurité du Travail du Québec. -SAX, N.I. Dangerous Properties of Industrial Materials. Toronto, Van Nostrand Reinold, 6e ed. 1984. -The Sigma-Aldrich Library of Chemical Safety Data, Edition II. -Guide de la loi et du règlement sur le transport des marchandises dangereuses au Canada. Centre de conformité international Ltée. 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 immediately.

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 catecholamines which may lead to cardiac arrhythmias. Do NOT use adrenergic agents such as epinephrine or pseudoephedrine.

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 375 mg/m ³ TWA 500 ppm IDLH	200 ppm TWA C 300 ppm	100 ppm TWA 375 mg/m ³ TWA 150 ppm STEL 560 mg/m ³ 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: Nitrogen 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 -

Toxicological Information

Carcinogenicity:

CAS# 108-88-3:

ACGIH: A4 - Not Classifiable as a Human Carcinogen

Section 11 -

Toxicological 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/96H Sunfish (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

Shipping Name	US DOT	Canada TDG
Hazard Class	Toluene	Toluene
UN Number	3	3 (9.2)
Packing Group	UN1294	UN1294
Other	II	II 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

M1003

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Effective Date: 9/07/2004

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/NDL: 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

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



Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
	Combustible material; avoid heat and sources of ignition. Harmful compound, minimize exposure. Irritating to skin, eyes, and the respiratory system. Dangerous for the environment	

Section I. Chemical Product and Company Identification

Chemical Name	1,3,5-Trimethylbenzene	Supplier	TCI America
Catalog Number	T0470		9211 N. Harborage St. Portland OR 1-800-423-8616
Synonym	Mesitylene	<div style="border: 2px solid black; padding: 5px;"> In case of Emergency Call </div>	
Chemical Formula	$(CH_3)_3C_6H_3$		
CAS Number	108-67-8		
			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 TOXICITY: Not 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. Risks of explosion of the product in presence of static discharge: Not available.	
Explosion Hazards	Combustible liquid. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, outgassing or explosion. Consult with local fire authorities before attempting large scale fire fighting operations.	

3/11/2005.

Appendix A-4. MSDS Information

0470	1,3,5-Trimethylbenzene	Page 3
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Section XII.	Ecological Information
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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 8.77×10^{-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
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Waste Disposal	Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve 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 local regulations when disposing of the substance.
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Section	XIV. Transport Information
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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
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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.

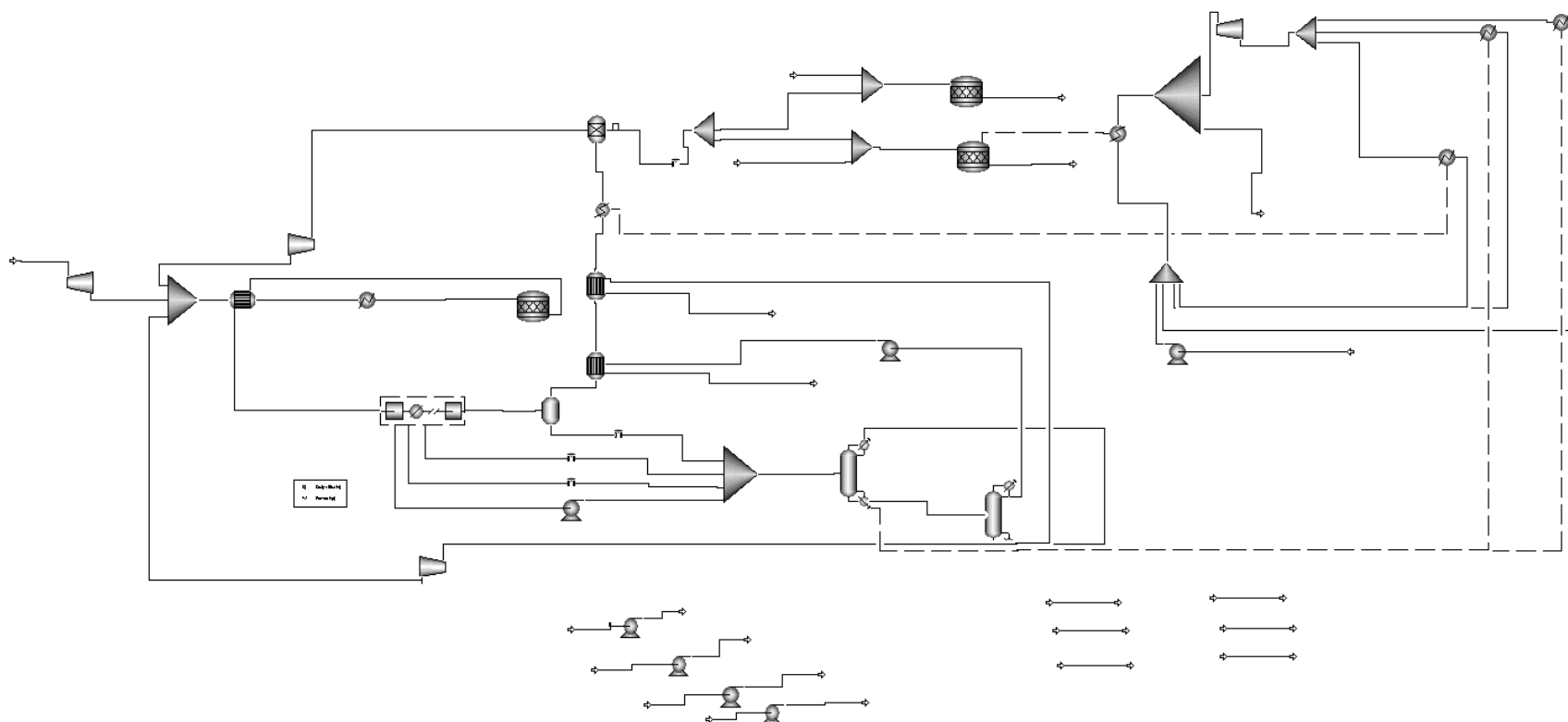
Printed 3/11/2005.

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

Printed 3/11/2005.

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

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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. 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

Appendix A-5. ASPEN Data

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	----

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

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
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Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

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

Appendix A-5. ASPEN Data

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					

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

Appendix A-5. ASPEN Data

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:					

Appendix A-5. ASPEN Data

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

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

Appendix A-5. ASPEN Data

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,

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

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

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

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

Appendix A-5. ASPEN Data

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					

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

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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
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S-409 S-410 S-411 S1 S2

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
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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

Appendix A-5. ASPEN Data

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 NUMBER	PRESSURE RATIO	MECHANICAL EFFICIENCY	ISENTROPIC 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 NUMBER	PRESSURE DROP PSI	TEMPERATURE 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

Appendix A-5. ASPEN Data

```

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

```

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

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-----
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

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

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****  INPUT PARAMETERS  ****

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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

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****  COL-SPECS  ****

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MOLAR VAPOR DIST / TOTAL DIST  1.00000
MASS REFLUX RATIO              0.10288
MASS DISTILLATE TO FEED RATIO  0.14001

```

```

****  PROFILES  ****

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P-SPEC      STAGE   1  PRES, PSIA      83.0000
              2      10.0000

```

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

```

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***  COMPONENT SPLIT FRACTIONS  ***

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```

                                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		HEAT DUTY BTU/HR
			LIQUID	VAPOR	
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		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	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		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	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					

Appendix A-5. ASPEN Data

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-

**** MOLE-Y-PROFILE ****						
STAGE	HYDROGEN	METHANE	ETHANE	ETHENE	PROPANE	
01	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-
02	15	0.11701E-21	0.20556E-02	0.20266E-01	0.12759E-02	0.69167E-
21	39	0.76572-197	0.77489E-42	0.44758E-27	0.22496E-30	0.20723E-
22	40	0.46289-204	0.17725E-43	0.40226E-28	0.16623E-31	0.33085E-
23	41	0.28420-211	0.40539E-45	0.36133E-29	0.12300E-32	0.52310E-
24	42	0.17907-218	0.91386E-47	0.30932E-30	0.87560E-34	0.76119E-

**** MOLE-Y-PROFILE ****						
STAGE	PROPENE	BENZENE	TOLUENE	P-XYL-01	1:3:5-01	
09	1	0.60559E-02	0.18969	0.18273E-01	0.17728E-03	0.32141E-
08	2	0.58149E-02	0.21555	0.25392E-01	0.36217E-03	0.11060E-
04	12	0.58932E-02	0.20310	0.24813E-01	0.18042E-02	0.96641E-
03	13	0.58980E-02	0.20263	0.24537E-01	0.17424E-02	0.25581E-
02	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-

**** 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	

Appendix A-5. ASPEN Data

	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
01	1	6.7728	0.25512	0.10703	0.42859E-01	0.18773E-
02	2	25.369	0.30349	0.97498E-01	0.29696E-01	0.95922E-
01	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
02	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-
03	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-
23	39	0.33751-206	0.10285E-44	0.43770E-29	0.16872E-32	0.52903E-
24	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-
25	42	0.86116-228	0.11438E-49	0.29698E-32	0.64741E-36	0.19071E-
**** MASS-X-PROFILE ****						
	STAGE	PROPENE	BENZENE	TOLUENE	P-XYL-01	1:3:5-01

Appendix A-5. ASPEN Data

07	1	0.49089E-03	0.75774	0.20522	0.57294E-02	0.26849E-
06	2	0.11868E-03	0.68266	0.29528	0.15932E-01	0.17053E-
01	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-

**** MASS-Y-PROFILE ****						
STAGE	HYDROGEN	METHANE	ETHANE	ETHENE	PROPANE	
01	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-
02	15	0.30016E-23	0.41963E-03	0.77545E-02	0.45548E-03	0.38811E-
21	39	0.19271-198	0.15520E-42	0.16803E-27	0.78792E-31	0.11409E-
22	40	0.11647-205	0.35493E-44	0.15098E-28	0.58208E-32	0.18210E-
23	41	0.71425-213	0.81082E-46	0.13546E-29	0.43020E-33	0.28758E-
24	42	0.44671-220	0.18143E-47	0.11510E-30	0.30398E-34	0.41538E-

**** MASS-Y-PROFILE ****						
STAGE	PROPENE	BENZENE	TOLUENE	P-XYL-01	1:3:5-01	
08	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-
03	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-
02	14	0.31578E-02	0.73414	0.10879	0.96203E-02	0.47061E-

Appendix A-5. ASPEN Data

```

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

```

Appendix A-5. ASPEN Data

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.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL		HEAT DUTY BTU/HR
			LIQUID	VAPOR	
1	249.71	35.000	21466.	36973.	- .25344+08
2	187.19	10.000	12043.	32583.	

Appendix A-5. ASPEN Data

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		FEED RATE			PRODUCT RATE	
	LBMOL/HR		LBMOL/HR			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		FEED RATE			PRODUCT RATE	
	LB/HR		LB/HR			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

Appendix A-5. ASPEN Data

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
DIFF.				RELATIVE
TOTAL BALANCE				

Appendix A-5. ASPEN Data

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-

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*** 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 NUMBER	REFERENCE COMPONENT	HEAT OF REACTION BTU/LBMOL
1	METHANE	-0.34514E+06
2	HYDROGEN	-0.10400E+06

REACTION EXTENTS:

REACTION NUMBER	REACTION 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

Appendix A-5. ASPEN Data

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			

Appendix A-5. ASPEN Data

```

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
COLD SIDE, 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 BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA 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	!	PRES	!	TEMP	!	VFRAC	!
!		!		!		!		!
!		!		!		!		!
!		!		!		!		!
!	BTU/HR	!	PSIA	!	F	!		!
!		!		!		!		!
=====								
!	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	!	PRES	!	TEMP	!	VFRAC	!
!		!		!		!		!
!		!		!		!		!
!		!		!		!		!
!	BTU/HR	!	PSIA	!	F	!		!
!		!		!		!		!
=====								
!	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      |
T= 2.4971D+02 |
1.3640D+02   |
P= 3.5000D+01 |
2.5000D+01   |
V= 0.0000D+00 |
0.0000D+00   |
|
S-212      <-----|
T= 1.2634D+02 |
1.0400D+02   |
P= 7.2000D+02 |
7.3000D+02   |
V= 1.0000D+00 |
1.0000D+00   |
----->|
HOT          |
|-----> S-215
|
T=
P=
V=
|
COLD          |
|<----- S-211
|
T=
P=
V=

```

DUTY AND AREA:

CALCULATED HEAT DUTY

BTU/HR

6478222.0023

Appendix A-5. ASPEN Data

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
COLD SIDE, 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 BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA 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      -----> |                | -----> 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      <----- |                | <----- 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
COLD SIDE, 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 BTU/HR	AREA SQFT	LMTD F	AVERAGE U BTU/HR-SQFT-R	UA 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	PRES	TEMP	VFRAC
BTU/HR	PSIA	F	
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      ! PRES      ! TEMP      ! VFRAC      !
!           !           !           !           !
!           !           !           !           !
! BTU/HR    ! PSIA      ! F         !           !
!           !           !           !           !
!=====+=====+=====+=====!
! 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

```

Appendix A-5. ASPEN Data

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

```

Appendix A-5. ASPEN Data

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

```

Appendix A-5. ASPEN Data

```

*** 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

```

Appendix A-5. ASPEN Data

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

```

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

```

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 NUMBER	REFERENCE COMPONENT	HEAT OF REACTION BTU/LBMOL
1	ETHANE	-31236.
2	ETHANE	61556.
3	ETHANE	44994.

Appendix A-5. ASPEN Data

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				

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

Appendix A-5. ASPEN Data

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

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INLET STREAMS:      S-102      S-104      S-103
OUTLET STREAM:      S-105
PROPERTY OPTION SET:  NRTL-RK   RENON (NRTL) / REDLICH-KWONG

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```

***  MASS AND ENERGY BALANCE  ***
                                IN          OUT          RELATIVE DIFF.
TOTAL BALANCE
  MOLE (LBMOL/HR)              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

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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			

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
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*** RESULTS ***

1	STREAM= S-221	SPLIT=	0.82431	KEY= 0	STREAM-ORDER=
2	S-220			0.17569	0

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 (Mass) from	Vapor (Mass) from	Liquid enthalpy	Vapor enthalpy	Liquid (Mass) flow	Vapor (Mass) flow
	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	196044 03	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 1.35×10^5 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](tel:+442073782841) |
sasha.maitala@jacobs.com <<mailto:sasha.maitala@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

<i>Parameter</i>	<i>Value</i>	<i>Comments</i>
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

<i>Vendor</i>	Babcock and Wilcox
<i>Boiler Capacity</i>	165,000 lb/hr
<i>Produced Steam Pressure</i>	100 psig
<i>Produced Steam Temperature</i>	Saturated
<i>Boiler Package</i>	FM120-112 Water Tube
<i>Pricing FOB point of fabrication</i>	\$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