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Process for Sustainably Sourced p-Xylene

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Process for Sustainably Sourced p-Xylene

Abstract

Demand for para-xylene, a feedstock used to produce polyethylene terephthalate (PET) plastics like those found in water bottles or textile fibers, has risen steadily.[14] In the PET market, there is a new sustainable focus, pushing producers to use environmentally-friendly processes to create plastic consumer products.[3] The current process to create para-xylene relies on fossil fuel cracking and reforming - a decidedly non-green process. This project follows a patent by GEVO, titled *Integrated Process to Selectively Convert Renewable Isobutanol to p-Xylene,* that explores a green process to convert isobutanol, created from biomass, to para-xylene.20 The raw material for this project is 500,000 tons of isobutylene per year, which is sourced from biomass and has already been converted from isobutanol. The design first feeds the fresh isobutylene, as well as the diluent isooctane, into the process. Isobutylene then oligomerizes over a zeolite catalyst, with a separation following to remove the undesired byproducts. While they are undesired in the process, these byproducts are trimers which can be a valuable coproduct, similar to GEVO's alcohol-to-jet fuel (ATJ).[4] The desired intermediate, 2,4,4-trimethylpentene, proceeds to another reactor and dehydrocyclizes over a chromium oxide doped alumina catalyst. Another separation occurs to isolate para-xylene and remove hydrogen. The final product stream is 89 wt% para-xylene. According to a financial analysis over a 10-year period, the process is currently unprofitable with a negative IRR. To be competitive in para-xylene markets and reach a 15% IRR, a 79% premium is necessary. This is unattractive for a standalone production facility, leading us to recommend that this plant should not be built. However, in the future as the push toward sustainable projects increase, this design may serve as a feasible and economic process for green para-xylene.

Disciplines

Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

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April 17th, 2018

Dear Dr. Sean Holleran and Professor Bruce Vrana,

The enclosed report contains a process design for converting isobutylene, sourced from biomass, into para-xylene. The process is fed 500,000 tons of isobutylene per year and creates 557 MM pounds of isobutylene per year in a product stream containing 89 wt% para-xylene. The design uses conditions from the GEVO patent titled *Integrated Process to Selectively Convert Renewable Isobutanol to p-Xylene*, as suggested in the project statement by Dr. Richard Bockrath. The design steps include an oligomerization reaction, a separation to remove byproducts, a dehydrocyclization reaction, a separation to obtain a pure product stream, a separation to remove hydrogen, and a recycle loop. This is competitive to the current process, which creates para-xylene through cracking, because of the high demand for a green process and the high purity in the final product stream.

From an economic standpoint, this process is currently unprofitable with a negative IRR. If marketing could negotiate a price premium for the product's sustainable benefits, they should seek a 79% premium to be competitive in the para-xylene market. This premium will ensure a 15% IRR and an NPV of $40,300. Though we do not recommend proceeding with the design with a standalone business case, we recommend incorporating the design into a marketable business plan that includes details on lowering the premium or research justifying the premium from a consumer-perspective, if possible. The report details the designs, analyses, and recommendations at each step of the process.

Thank you for your guidance throughout this project.

Sincerely,

Grace Memmo	John Calhoun Newlon	Xiaoxin Tang
____________________	____________________	____________________

Process for Sustainably Sourced p-Xylene

By: Grace Memmo, John Calhoun Newlon, Xiaoxin Tang

Projected submitted to Dr. Sean Holleran and Prof. Bruce Vrana

Project proposed by Dr. Richard Bockrath

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Glossary

Word	Abbreviation
para-Xylene	p-Xylene
meta-Xylene	m-Xylene
ortho-Xylene	o-Xylene
Chromium oxide doped alumina catalyst	Cr/Al_2O_3
Polyethylene Terephthalate	PET
2,4,4-trimethylpentene	TMP
BTX	mixtures made of benzene, toluene, and the xylene isomers
Dimethyl Furan	DMF
Alcohol-to-Jet Fuel	ATJ
Weight hourly space velocity	WHSV
Log Mean Temperature Difference	LMTD

Section 1 Abstract

Demand for para-xylene, a feedstock used to produce polyethylene terephthalate (PET) plastics like those found in water bottles or textile fibers, has risen steadily.[14] In the PET market, there is a new sustainable focus, pushing producers to use environmentally-friendly processes to create plastic consumer products.[3] The current process to create para-xylene relies on fossil fuel cracking and reforming - a decidedly non-green process. This project follows a patent by GEVO, titled *Integrated Process to Selectively Convert Renewable Isobutanol to p-Xylene*, that explores a green process to convert isobutanol, created from biomass, to para-xylene.[20] The raw material for this project is 500,000 tons of isobutylene per year, which is sourced from biomass and has already been converted from isobutanol. The design first feeds the fresh isobutylene, as well as the diluent isooctane, into the process. Isobutylene then oligomerizes over a zeolite catalyst, with a separation following to remove the undesired byproducts. While they are undesired in the process, these byproducts are trimers which can be a valuable coproduct, similar to GEVO's alcohol-to-jet fuel (ATJ).[4] The desired intermediate, 2,4,4-trimethylpentene, proceeds to another reactor and dehydrocyclizes over a chromium oxide doped alumina catalyst. Another separation occurs to isolate para-xylene and remove hydrogen. The final product stream is 89 wt% para-xylene. According to a financial analysis over a 10-year period, the process is currently unprofitable with a negative IRR. To be competitive in para-xylene markets and reach a 15% IRR, a 79% premium is necessary. This is unattractive for a standalone production facility, leading us to recommend that this plant should not be built. However, in the future as the push toward sustainable projects increase, this design may serve as a feasible and economic process for green para-xylene.

Section 2
Introduction and Objective Time Chart

Section 2.1 Introduction

para-Xylene (p-xylene) is an aromatic hydrocarbon, distinguished from the meta-xylene (m-xylene) and ortho-xylene (o-xylene) isomers of ethylbenzene by the substituent positions of its methyl groups. Normally produced through the catalytic reforming of petroleum naphtha, the p-, m-, and o- xylenes are all significant feedstocks in industry. However, their use and value are limited by their individual purity in any given stream, and their low relative volatilities make separation difficult.

With that in mind, research has been done on finding efficient methods to increase the selectivity for p-xylene. p-Xylene is the most valuable of the xylene isomers for commercial processes creating PET, while o-Xylene is used in the production of phthalic anhydride, and m-Xylene is used in the production of isopthalic anhydride.[23,29] Recent research has proposed several improvements to existing processes and has identified new catalysts that promote conversion to p-xylene over its isomers.[12] Several of these pathways source from biomass, offering sustainable p-xylene in competitive yields. The increasing growth of demand for products built primarily from p-xylene's derivatives, the competitive pressures to reduce production costs, and the consumer push to develop sustainable products are all promising for further innovation. Our green process incorporates innovation where it has been sufficiently tested, but the production of p-xylene remains expensive and energy-intensive.

Our goal is to design a 30-year plant that creates p-xylene. The design closely follows GEVO's patent, *Integrated Process to Selectively Convert Renewable Isobutanol to p-Xylene*, which proposes several catalytic mechanisms that convert green isobutanol to p-xylene.[20] Our process is fed 500,000 tons of isobutylene per year, sourced from biomass. Because isobutylene is already the raw material, examples in the patent discussing the conversion of isobutanol to isobutylene were ignored. We specifically used Examples 7, 13, and 16 for their relatively high purities and optimal operating conditions. The process includes two reactions. First, an oligomerization reaction converts isobutylene into 2,4,4-trimethylpentene (TMP) over an HZSM-5 catalyst. Second, a dehydrocyclization reaction converts TMP into xylene isomers over a chromium oxide doped alumina catalyst (Cr/Al_2O_3), which enhances selectivity to p-xylene.

The xylene separation process is intensive, often requiring over 200 stages, because of the isomers' strong affinity to produce eutectic mixtures and close relative volatilities. Due to the difficulty and scale of this separation, independent xylene purification plants were created. Our product stream of 89 wt% p-xylene is sent to these plants to be processed in order to obtain pure p-xylene.

p-Xylene is principally used to synthesize terephthalic acid, which is esterified with ethylene glycol to produce polyethylene terephthalate (PET).[20] This thermoplastic resin is widely used for plastic bottles, liquid and food containers, and fibers.[30] Because the bottles take a long time to biodegrade and are often not properly recycled, they compose large proportions of landfills and marine garbage gyres. These bottles are primarily composed of PET, so any premium levied on the green p-xylene would comprise a significant premium on the plastic bottles as well, which makes penetrating that market difficult. However, over 60% of PET made is spun into fibers for clothing.[30] Because PET makes up less of the total material used in clothing, and clothing markets are more sensitive to consumer needs, we believe customers would more readily accept the premium.

The plant will produce 557 MM lb/yr of p-xylene in an 89 wt% p-xylene stream. A coproduct stream, rich in longer hydrocarbons commonly used for jet fuels and diesels, will also be sold. Other byproducts will be recycled or consumed internally to increase efficiencies. The plant will be located in Iowa, in close proximity to our company’s isobutylene plant, the xylene purification centers, and green raw material.

Section 2.2 Objective Time Chart

Name of Project: Process for Sustainably Sourced p-Xylene

Project Author: Dr. Richard Bockrath

Project Advisors: Dr. Sean Holleran and Professor Bruce Vrana

Project Leaders: Grace Memmo, John Calhoun Newlon, and Xiaoxin Tang

Specific Goals:
- Design a plant to convert 500,000 tons of sustainably sourced isobutylene to higher value products
- Create a crude xylene product that is 90 wt% para-xylene

Project Scope:

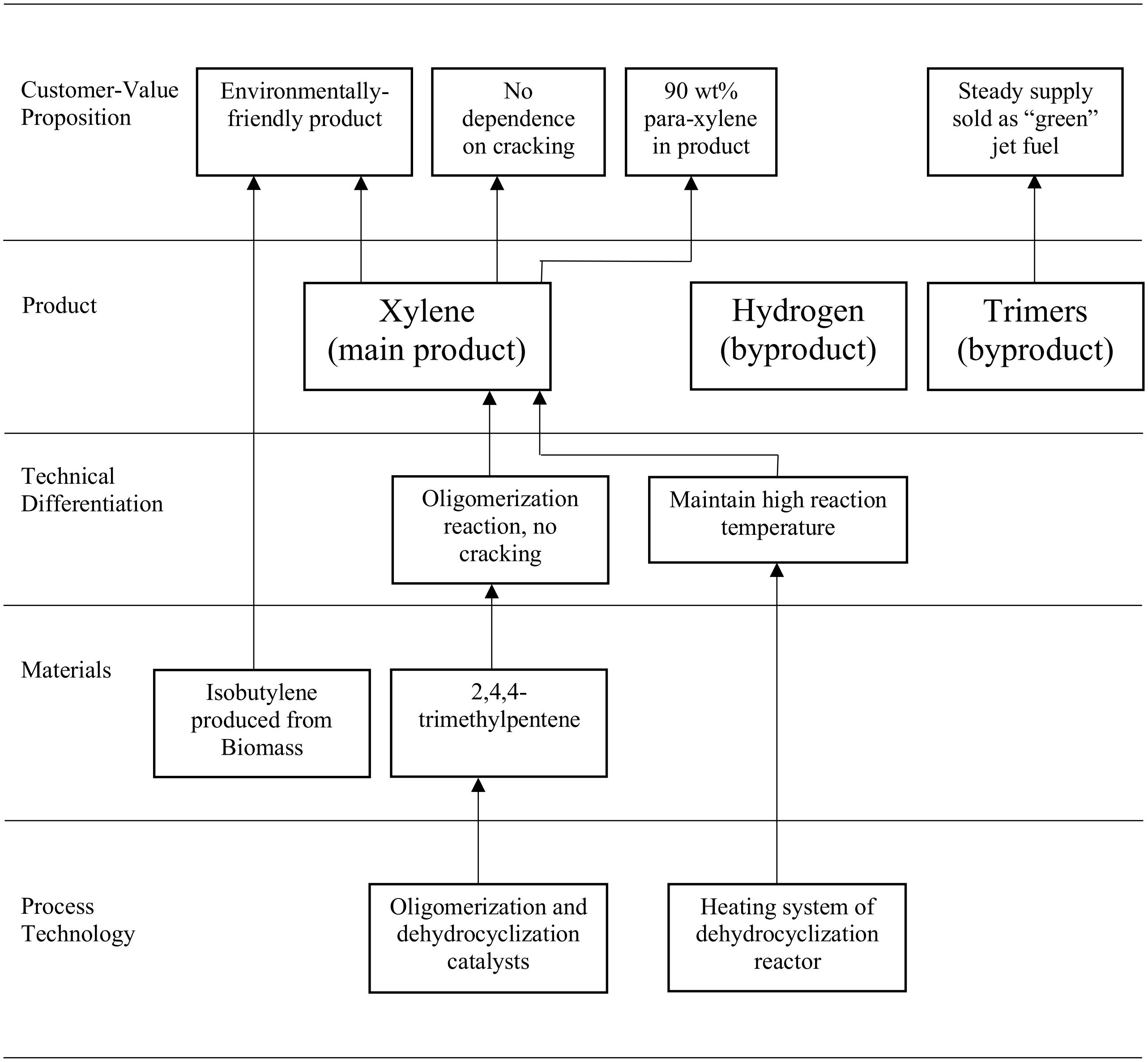
In Scope
- Convert 500,000 tons of isobutylene into para-xylene
- Product a 90 wt% para-xylene crude product
- Design process, including all equipment and process conditions
- Size and cost all equipment
- Include catalyst regeneration process
- Analyze profitability and economics of project by calculating cost of plant and required pricing premium of product

Out of Scope
- Creation of isobutylene
- Separation of xylene product to obtain pure para-xylene
- Testing of patent and assumptions
- Design of process control system
- Kinetic data of catalysts

Deliverables
- Flowsheet of process and simulation results
- Mass and energy balances
- Equipment design
- Cost of plant
- Economic and profitability analysis to understand feasibility of project
- Written report and presentation describing project

Timeline
- Mid-semester presentation on February 27, 2018
- Final report due on April 17, 2018
- Final presentation on April 24, 2018

Section 3 Innovation Map



Section 4
Market and Competitive Analysis

The market for p-xylene has consistently grown for decades as consumers demand more goods made of PET.[29] Efforts to improve production efficiency have focused on the process, rather than the product, so the existing market is largely shaped by purity and quantity requirements.

The p-xylene market is principally supplied by the major oil producers. These companies produce a large amount of BTX (mixtures made of benzene, toluene, and the xylene isomers) from naphtha hydrotreating. This excess BTX justifies in-house reforming of BTX crudes into either xylene crude streams or commercial grade p-xylene.[12] Because p-xylene is such a chemically-stable feedstock, it has historically supported a market in contango, where short-term supply exceeds short-term demand. Producers are currently responding to increased demand from the PET market, largely led by plastic fibers, by increasing supply and storage capabilities. While the established oil producers are well-posed to increase production of p-xylene from petroleum feedstocks, they are ill-suited to capture any growth in green markets. Additionally, Research on the economic value of sustainability as a product offering has shown that customers are reluctant to buy products marketed as eco-friendly from companies entrenched in other ventures that are decidedly unsustainable.[17]

The high purity of our product is also notable. p-Xylene is more valuable when it can be more readily converted to its end-products, but it is currently sold in large quantities at significantly lower purities.[2] Designs that improve conversion and selectivity not only increase the value of the product stream, but also reduce the cost of post-production processing and storage. While this does require more capital investment for reactor technology and catalysts to exploit more selective reaction mechanisms, the 30-year lifespan of the isobutylene feed justifies these expenses so as to improve long-term returns.

To sell green products in an already competitive market, a premium will be added to the cost of the products. Many studies have evaluated how high of a premium consumers are willing to pay for a green product. In 2012, McKinsey & Company surveyed 1,000 consumers in Europe and the United States.[15] More than 70% of those surveyed would be willing to pay a 5% premium on products, as shown in Figure 4.1. As expected, the willingness to pay decreases as the premium increases. However, in the category of packaging, 10% of consumers said they would be willing to pay a 25% premium on these products. p-Xylene's uses are in packaging, so this is significant to note for this process.

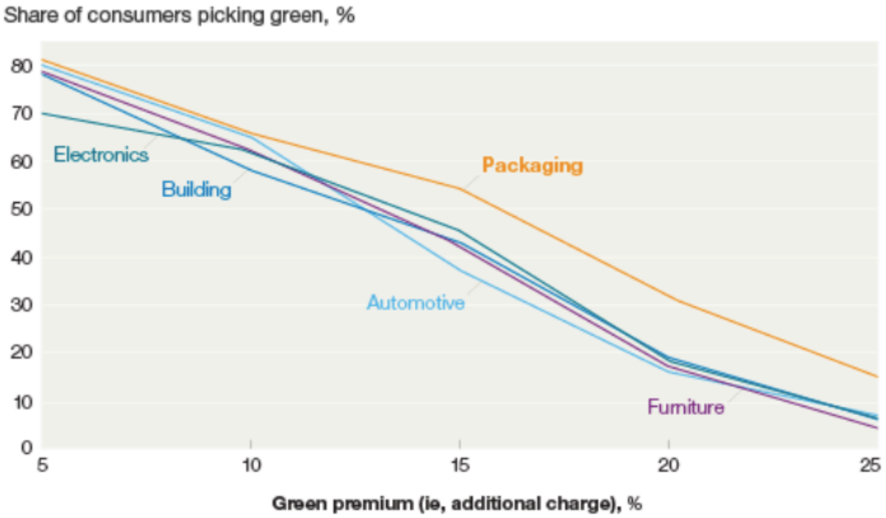


Figure 4.1 Graph of a green premium percentage versus the percent of customers surveyed willing to pay the premium.[15] As shown, 70% of customers will pay a 5% premium. All categories, except for packaging, decrease at the same rate. 10% of customers are willing to pay a 25% premium on packaging.

Other sources have shown that the number of consumers willing to pay a premium has increased throughout the years. A 2015 Nielsen survey of 30,000 people around the world shows that 66% of those surveyed are willing to pay more for sustainable goods, an increase from 55% in 2014 and 50% in 2013.[3] This steady increase is promising for our product. Furthermore, the survey states that 73% of millennials are willing to pay for sustainable offerings. Nestlé chairman, Peter Brabeck-Letmathe, told CNBC in 2016 that "If you look at the millennials, they are the first generation now who are willing consciously to spend more for better quality, for sustainability, for traceability."[8] Because we will need to sell our product with a premium, these studies confirm that there is a market available for green products and that there is a push for sustainability from the customer.

While the sustainable nature of the isobutylene as a biomass product significantly increases the value of this p-xylene, the production process remains inefficient. To reach a customer as a tangible product, p-xylene requires further processing and other feedstocks that will be difficult to source sustainably, which could weaken the value proposition of the product as "sustainable." Even internally, the design requires very large annual energy consumption, which would be difficult to supply to a plant in the Midwestern United States from renewable sources such as wind or solar power. Though there potentially is a huge value for a new entrant to meet growing demand for customer goods with sustainable production, further work is necessary to determine which simultaneous processes integral to PET fibers can be designed sustainably. As the future of environmental policy and green markets unfold, a watchful eye will know if and when the demand exists for sustainably sourced p-xylene and how to meet it.

Section 5
Customer Requirements

As a stable chemical feedstock, p-xylene's fitness-to-standard[24] is largely determined by production rate and purity. This design can annually produce about 279,000 tons of p-xylene from 500,000 tons of isobutylene. While there are no universal standards or gradations for xylene stream purity, product value is diminished by impurities depending on their relative ease of separation in later processing. This design aims to create a stream of 90 wt% p-xylene, decreasing separation costs and increasing the amount of valuable p-xylene.

New-unique-difficult[24] variables are largely shaped by the green nature of our product and the complexities associated with sustainably-sourced goods. End-user goods often seek official external certification to bolster claims of sustainability, and stricter certifications are more valuable to customers. There are no widely-used certifications for sustainably-sourced clothing, so the biomass nature of the isobutylene might be sufficient for green marketing downstream, but more stringent qualifications would require review of the process design as well.[7] While the emissions and purification processes are designed to meet or exceed safety and environmental regulations, they are not designed to use sustainably-sourced energy or intermediates.

Section 6
Critical-to-Quality Variables

N/A

Section 7
Product Concepts

N/A

Section 8
Superior Product Concepts

N/A

Section 9
Competitive Patent Analysis

As suggested in the problem statement, a patent filed by GEVO was used for the process design. GEVO patent US2011/0087000A1, titled *Integrated Process to Selectively Convert Renewable Isobutanol to p-Xylene*, describes a green process in detail to create p-xylene. Because of the growth in bio-based fuels and the high value of p-xylene, other companies in addition to GEVO have created pilot plants to produce bio-based p-xylene. While we explored other patents, the GEVO patent stated above was used because its raw material, isobutanol sourced from biomass, is converted to isobutylene, the raw material for our process. Another patent focusing on a green process and using a similar feedstock is *Renewable Para-Xylene From Acetic Acid* US2014/0121430A1 from Archer Daniels Midland Company in 2014. This patent has fewer details, and the examples and information are the same as the GEVO patent.[25]

There are also patents that explore a higher purity product stream but are not green. For example, a Honeywell patent, US2008/0287719A1 titled *Process of Para-xylene Production from Light Aliphatics*, describes a similar process to the GEVO patent to make p-xylene from butane; however, butane is not sourced sustainably.[12] Like the GEVO patent, butene first dimerizes, with a side reaction producing trimers. Then, the desired dimers are aromatized to create a p-xylene mixture. This patent explores several different reactor conditions and catalysts with corresponding p-xylene purity and TMP conversion. Like the GEVO patent, one trial yields a 90.4 wt% purity p-xylene stream; however, the conversion of TMP is only 25.6%. While this patent shows a process to create a higher purity product stream than the traditional cracking processes, the fact that the raw material is not sustainably sourced removes it from being a competitor in our project's market.

Another patent by Honeywell, US2010/0331568A1 titled *Carbohydrate Route to Para-Xylene and Terephthalic acid*, discusses creating p-xylene from 2,5-dimethyl furan (DMF).[1] DMF is sourced from synthesizing carbohydrates, ensuring renewable feedstocks for the process. Unlike the GEVO patent, this method creates product streams with very low fractions of p-xylene. While the GEVO patent is better suited for our project due to the starting material and higher product purity, the process described in this Honeywell patent is competitive to ours due to the sustainably-sourced raw material.

The main competitors of this project product-wise are the companies creating p-xylene by cracking conventional petroleum-based feedstocks. While these pathways are not green because their feedstocks contribute to environmental degradation, the patents on these processes were explored for purity comparisons. Two patents from ExxonMobil, US2002/0082462A1 titled *Process For Production of Paraxylene* and US2010/0040517A1 titled *Process of Manufacturing Para-Xylene* were studied.[6,2] The first patent does not state the exact purity, conversion, or selectivity, but it does mention a process flaw where a significant amount of p-xylene is lost in the isomerization step. The latter describes a process that manufactures p-xylene from a pygas feedstock. It states that common processes for creating p-xylene from petroleum feedstock only has a maximum product stream purity of only 50%, far lower than our goal. From these patents, it is clear that high purity p-xylene is scarce when sourced from petroleum feed.

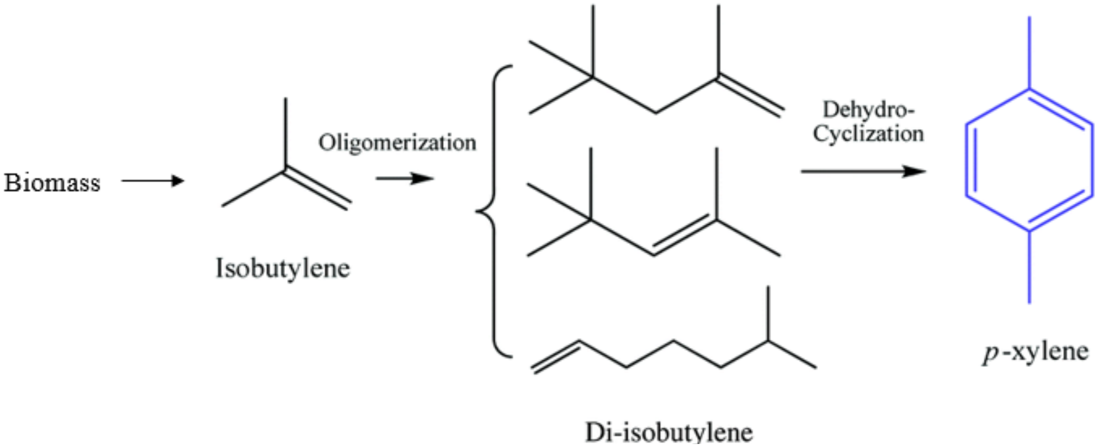
Section 10
Preliminary Process Synthesis

Section 10.1 Reactions

The goal of the project is to convert 500,000 tons of isobutylene, sustainably sourced from biomass, into a crude product with at least 90 wt% p-xylene. The other 10% can include the isomers of p-xylene: m-xylene and o-xylene. The process requires two reactions:

$$2C_4H_8 \rightarrow C_8H_{16} \qquad (1)$$

$$C_8H_{16} \rightarrow C_8H_{10} + 3H_2 \qquad (2)$$



(2,4,4-trimethylpentene)

Figure 10.1.[16] Isobutylene, sourced from biomass, undergoes an oligomerization reaction to create 2,4,4-trimethylpentene (TMP). TMP then undergoes a dehydrocyclization reaction to create p-xylene.

The first reaction is an oligomerization reaction converting liquid isobutylene, the main raw material, into liquid TMP, an intermediate. The reaction is exothermic with a heat of reaction of -13,350 BTU/lbmol. The conversion of isobutylene to TMP is 60%. There is a side reaction that converts 30% of the isobutylene into trimers and tetramers.[20] It will be important to separate out these large compounds immediately after the first reaction, so they do not contaminate the final product. In the patent, only 2% of the isobutylene was converted into tetramers, so for simplicity, the tetramers have been ignored. The other 10% of isobutylene is unreacted. This reaction requires a diluent for kinetic reasons to suppress the trimer and tetramer reactions by reducing the probability of the dimer (TMP) bonding to the monomer (isobutylene) and to increase the selectivity of TMP.[20] While the patent suggested many diluents, isooctane was chosen because it is inert, acts as a modifier to prevent further polymerization, and can be used as a diluent in the second reaction (stated below). Lastly, the first reaction requires a catalyst; HZSM-5 was chosen due to example trials stated in the patent.

The second reaction, a dehydrocyclization reaction, converts the intermediate TMP into the desired product, p-xylene. The reaction is endothermic with a heat of reaction of 55,215 BTU/lbmol. Only about 42% of the overall TMP is converted; 38% is converted to p-xylene and 4% is converted to m-xylene and o-xylene, the undesirable isomers of p-xylene, evenly.[20] Hydrogen is produced as a side product, which must be removed from the system because hydrogen buildup slows reaction rates. Isooctane is used as a diluent to reduce coking of the catalyst. Lastly, a chromium oxide doped alumina catalyst (Cr/Al_2O_3) was chosen due to example trials from the patent. The catalyst cokes easily, so the coke will need to be burned off frequently (see Section 13.4.2.).

Table 10.1: Reactions in the Oligomerization (1) and Dehydrocyclization (2) Reactors. This table shows which reactor each reaction occurs in, the reaction, the products made, and the fractional conversion obtained from the patent. The heat of reaction shows that the reactions are exothermic in the first reactor and endothermic in the second reactor.

Reactor	Reaction	Products	Fractional Conversion (%)	Heat of Reaction (BTU/lbmol)
1	$2C_4H_8 \rightarrow C_8H_{16}$	TMP	60	-15,350
1	$3C_4H_8 \rightarrow C_{12}H_{24}$	Trimers	30	-16,018
2	$C_8H_{16} \rightarrow C_8H_{10} + 3H_2$	para-Xylene	37.8	55,215
2	$C_8H_{16} \rightarrow C_8H_{10} + 3H_2$	meta-Xylene	2.1	55,666
2	$C_8H_{16} \rightarrow C_8H_{10} + 3H_2$	ortho-Xylene	2.1	54,910

Section 10.2 Patent Information

Most information about the specific process conditions were obtained from the patent. The first step of the patent converts isobutanol to isobutylene; however, the process design in this report has a feed of isobutylene, so this step was ignored. To decide which pilot plant trials to follow in the patent, process conditions and final purity were taken into account. As far as process conditions, most examples showed running the second reactor under vacuum, which is very capital-intensive and difficult. Example 13 documents a trial running the reactor at atmospheric pressure, so these conditions were chosen. Example 13 follows Example 7, which states conditions for the first reactor. Example 7 follows Example 3, which was ignored because it discusses converting isobutanol into isobutylene.

Example 7 states that liquid isobutylene entered a fixed-bed oligomerization reactor packed with a ZSM-5 catalyst. While many catalysts can be used, ZSM-5 was chosen for this project based on this example. Additionally, the reactor conditions were 347ºF and 750 psig. The WHSV was 15 hr^{-1}, which was used later to find the amount of catalyst needed. Lastly, the conversions stated in the section above were found in the example.

Example 13 states the reactor conditions for the dehydrocyclization reactor. It first explains that trimers and tetramers were removed from the reactor effluent. The example then states that nitrogen diluent gas was fed to the second reactor. This is ignored in our design because we are using isooctane as the diluent, as explained above. The fixed bed reactor used a Cr/Al_2O_3 catalyst. The reactor conditions were 1022ºF and atmospheric pressure. The WHSV was 1.1 hr^{1}, which was used later to find the amount of catalyst needed. Lastly, this example did not state conversions for the reactions, so Example 16 was utilized because it had the complete integrated system.

There were many options about the locations of separations and recycling to obtain a high purity product and to decrease the flow rate into subsequent equipment. The patent suggested to remove trimers after the first reactor. This was followed to decrease the flow rate in the second reactor and remove an undesired byproduct that could then be sold as a valuable product. The patent also includes a recycle loop to recover any unreacted reactant and recover diluent. It suggests having two recycle streams: one sending isobutylene to the feed of the first reactor and one sending isooctene to the feed of the second reactor. These separations were considered as explained below. Separation of the final stream to obtain 100% purity of p-xylene is out of scope of the project. The final stream will be sent to another plant to separate for a fixed cost.

Section 10.3 Initial Considerations and Alternative Designs

The flow rate of isobutylene was calculated to be 126,820 lb/hr, due to the manufacturing plant's need to convert 500,000 tons per year (from the problem statement) and the industry standard that plant uptime is 90% of the year. Due to this large flow rate, it was realized that this plant would be very large-scale with high flow rates. Therefore, the plant needs very large equipment and will be capital-intensive. The equipment diameter should be no larger than 18 feet to be transported on the highway. If equipment will be transported by barge, it can be 20 feet in diameter and 60 feet in length. Any larger equipment will need to be assembled on site. The plant will be situated along the Mississippi River in Iowa. We decided on this location because the company's plant already exists there to make isobutylene from biomass, due to the large production of corn in the Midwest. Additionally, the xylene separation plant will be close by.

Alternatives designs stated below were eliminated based on financials and product purity. First, different separation locations were considered. It was determined that a separation should occur after the first reactor to remove trimers, as opposed to after the second reactor. There are many reasons for this: the flow rate into the second reactor will decrease, reducing the size of the reactor; future separation can occur more easily because there will be fewer components; and a pure trimer stream can be sold. Another separation should occur after the second reactor to separate out the product and remove hydrogen from the system. Separations are fairly difficult due to the similar boiling points of TMP (210ºF), isooctane (212ºF), and xylene (280ºF) at atmospheric pressure, so it was realized that a large distillation column would be required. Thirdly, there was a discussion about separating out the hydrogen stream even further because reactants and diluents were being removed from the system through the hydrogen stream, and hydrogen can slow reaction rates. The cost of a compressor, condenser, and flash drum for this additional separation equates to \$3.85 MM, a price largely influenced by the cost of the compressor. Without this flash, 72.9 MM pounds of isooctane are lost per year, so an additional \$12.4 MM per year would be spent on fresh isooctane to add to the system. There are also intangible losses of isobutylene, TMP, and p-xylene. We decided that recovering the extra hydrogen would be worth it based on this cost benefit analysis. This additional separation was included in the final design.

There was a focus on the design of the second reactor due to the fast coking nature of the Cr/Al_2O_3 catalyst and the fact that the reactor is run at 1022ºF, a high temperature. First, it was suggested that the reactors be shell-in-tube reactors. This posed an issue because heating the tubes, filling the tubes with over 1.5 MM pounds of catalyst, and cleaning out the coke from the tubes would be extremely difficult. This type of reactor would also be very expensive. Instead, a packed bed reactor was designed. A heat exchanger placed before the reactor will heat the fresh stream, and a fired heater placed in the recirculation loop around the reactor will heat the reactor effluent. This recirculation is explained later. Instead of a fired heater, the use of molten salt to heat the reactor was also considered. This was dismissed because of the difficulty of handling molten salts.

Furthermore, the size of the reactor needed to be evaluated. Because of the large size of the stream entering the reactor and the large amount of catalyst, there would need to be multiple reactors in order to keep the L/D ratio reasonable. Originally, the reactors were going to be in series; however, the design was switched to parallel to remove the need of fired heaters between each reactor. For the catalyst regeneration process, consultants suggested using a swing reactor that would undergo decoking, allowing continuous regeneration of the catalyst and preventing a shutdown every time decoking needed to occur. A swing reactor is very valuable due to the fast coking time of the catalyst. This reactor set-up is further discussed in Section 13.4 and 15.4.

After first running the process, it was realized that the low conversion in the second reactor, along with the adiabatic temperature drops and rises, would pose issues for a high purity product and stable process conditions. Therefore, recirculation loops were added to both reactors to improve conversion and achieve the conditions of an isothermal reactor. The first reaction is exothermic, so heat needs to be removed from the stream. The second reaction is endothermic, so heat needs to be added to the stream. The adiabatic temperature rise and drop of the first and second reactor, respectively, were calculated and found to be reasonable and avoid process safety issues. Additionally, the main reason for the recirculation loop in the second reactor is to improve conversion. The TMP in the second reactor only has a single-pass conversion of 42%. By sending the stream through multiple times, the overall conversion is improved. Because the patent does not state any information about the reaction being reversible, it is assumed that the reactions are not equilibrium-limited and will not be affected by product entering the reactor. A recirculation loop requires a larger reactor to handle the total amount of material that is recycled back into the reactor with the fresh feed. This disadvantage increases the cost of the reactor and the amount of catalyst needed greatly. We optimized the reactor size by correlating the amount recycled with the final product purity. While a smaller reactor decreases the equipment cost, a less pure product increases the downstream separation cost. We were able to decrease the split for both reactors from the original amount used and still obtain a high purity to a certain extent. These optimized values were used in the final flowsheet.

It was also debated where the recycle loop should enter the process. A recycle loop is required to recover unreacted reactant and diluent. At first, it was thought that a recycle loop would reconnect at the beginning of each reactor. Then, after recirculation loops were included for each reactor, it was decided that the recycle loop would simply connect back to the beginning of the process and mix with the fresh isobutylene and isooctane feeds.

As far as diluents, isooctane is used in the final design. The patent states that a diluent should be used in the first reactor to provide selective dimerization of isobutylene, the C_4 alkene. After assessing different diluents suggested by the patent based on their cost and how they would affect the process, it was decided that isooctane would be the diluent for the first reactor. The patent stated that 20-90% of the feed to the oligomerization reactor should be diluent; this design specification was followed in the simulation. For the second reactor, isobutylene was initially chosen because it is the main raw material, so it would be a cost-savings opportunity. However, consultants suggested that isobutylene is too reactive, and an inert component should be used in the second reactor. Because the patent also suggested isooctane and it was being used for the first reactor, isooctane was chosen. A diluent is used in the second reactor to improve selectivity of p-xylene and to suppress cracking.

The addition of a turbine was considered in the stream exiting the first reactor to try to recover work from the large decrease in pressure from the reactor outlet at 750 psig to the distillation column inlet at 65 psig. After adding a turbine, ASPEN calculated that only 91 hp would be recovered. This value is small due to the fact that the stream is liquid. The cost of a turbine would not outweigh the work recovered; therefore, a simple valve will be installed to decrease the pressure.

The patent states that trimers will be formed in the first reaction but does not specify which trimers. Because isobutylene is the raw material, we decided to use a trimer that had a similar chemical formula with only carbons and hydrogens. Therefore, we picked 1-dodecene as a proxy compound to model all trimers.

Section 10.4 Cr/Al_2O_3 Catalyst Regeneration

The regeneration process of decoking the Cr/Al_2O_3 catalyst requires a combustion reaction. Research suggests that a stream made of 1% oxygen should be introduced to the reactor.[21] To create this stream, 95 parts of nitrogen should be mixed with 5 parts of air. If fresh streams were constantly fed to the reactor, 810 MM pounds of nitrogen would be required. This would cost $8 MM per year. Industrial consultants suggested installing a recycle loop to decrease the amount of fresh nitrogen needed and to cut costs. This recycle loop works because the gases exiting the decoking process are mostly nitrogen and a small amount of carbon dioxide. A purge should be installed to remove the carbon dioxide. If 10% is purged and the rest is recycled back, the new stream entering the reactor will be 85% recycled gas with 5% pure air and 10% fresh nitrogen. Instead of fresh nitrogen making up 95% of the stream, it now only makes up 10%, reducing the fresh nitrogen feed by 85%. A blower will need to be added in to recycle the exit gas back to the front of the reactor. Compared to the alternative of spending $8 MM on nitrogen per year, this will be more economical and followed for this project.

Section 11
Assembly of Database

Section 11.1 Cost of Chemicals

The two main raw materials are isobutylene and isooctane. The project statement says that the isobutylene will be purchased from another process in our company for 90% of the nominal market price at \$0.75/lb.[18] Isooctane will be purchased for \$0.17/lb from Chevron Phillips.[11] The cost of utilities – cooling water, chilled water, steam, electricity, and refrigeration – were taken from standard guidelines[24] (see Tables 19.2 for costs). The already existing on-site cooling tower will be used. Nitrogen will be purchased at \$0.01/lb to purge the system with nitrogen for flammability concerns and to decoke the reactor.[10] The cost of air for the decoking process is negligible, and we will use the air system on site. Lastly, methane, used as fuel for the fired heater, will be purchased for \$5.00/1000 SCF from Airgas.[28]

The two products are p-xylene and trimers. According to the project statement, a 2016 report by Grand View Research states that the cost of p-xylene in 2015 was \$0.79/lb and will rise to \$0.86/lb by 2024.[19] Because this is the market price on delivery, the selling price we used was less than this amount due to the fact that our stream requires downstream processing and freight. Therefore, the selling price used for this project was \$0.75/lb. Trimers will also have a selling price as green jet fuel of \$0.15/lb. This value was obtained from correspondence with Honeywell about their prices of biodiesels and green jet fuels.

Section 11.2 ASPEN Simulation

The chemical process modeling was done in ASPEN, which supplied relevant thermodynamic and kinetic data using the NRTL method, which was selected to best model the eutectic nature of xylene crudes. The reaction mechanisms were sourced from GEVO's patent but were limited in their description of relevant thermodynamic and kinetic data, constraining the reactor model to RSTOIC. Further research on these processes, as well as additional scale-up to pilot plants, would allow for more precise estimates of energy demands and catalyst regeneration, which could ultimately influence project economics. The columns were modeled by DSTWU, the flash drum was modeled by FLASH, and all but one of the heat exchangers were modeled by HEATER for simplicity. One heat exchanger used HEATX because it had two process streams entering and exiting it. Operating conditions for the reactor were taken from the patent, and the heat exchangers and compressors changed the temperatures and pressures of the streams to those conditions. The conditions for the distillation columns were determined based on design specifications on purity and bottoms temperature by changing the bottoms rate and the reflux ratio.[10] The conditions for the flash drum were based on the boiling points. To achieve successful operation of the flash drum, hydrogen was changed to a Henry's component. Lastly, storage tanks were added separately from the simulation due to their need in a real manufacturing plant.

Section 11.3 Chemical Properties

The MSDS sheets for all of the chemicals used in the process can be found in Appendix 25.4 Any considerations taken based on safety were determined based on the chemical properties in the MSDS sheets. Tables 11.1 and 11.2 show property data of all major chemicals and utilities.

Table 11.1 Properties of Major Chemicals in the Process

Chemical	**Molecular Weight (lb/lbmol)**	**Heat Capacity (BTU/lb•°F)**	**Density (lb/ft^3)**	**Important Notes**
Isobutylene	56.1	0.64	35.2	Extremely Flammable
Isooctane	114.2	0.52	43.0	Very Flammable, toxic to aquatic life, can be fatal if ingested
TMP	112.2	0.52	43.2	
Trimer	168.0	0.48	46.2	
p-Xylene	106.2	0.41	52.0	
m-Xylene	106.2	0.41	52.2	
o-Xylene	106.2	0.43	53.1	

Table 11.2 Properties of Utilities in the Process

Material	**Supply Temperature (°F)**	**Heat Capacity (BTU/lb•°F)**	**Latent Heat of Fusion (BTU/lb)**
Cooling Water	86	0.999	-
Chilled Water	45	0.999	-
150 psig Steam	366	-	857
1250 psig Steam	574	-	577

Section 11.4 Catalyst Properties

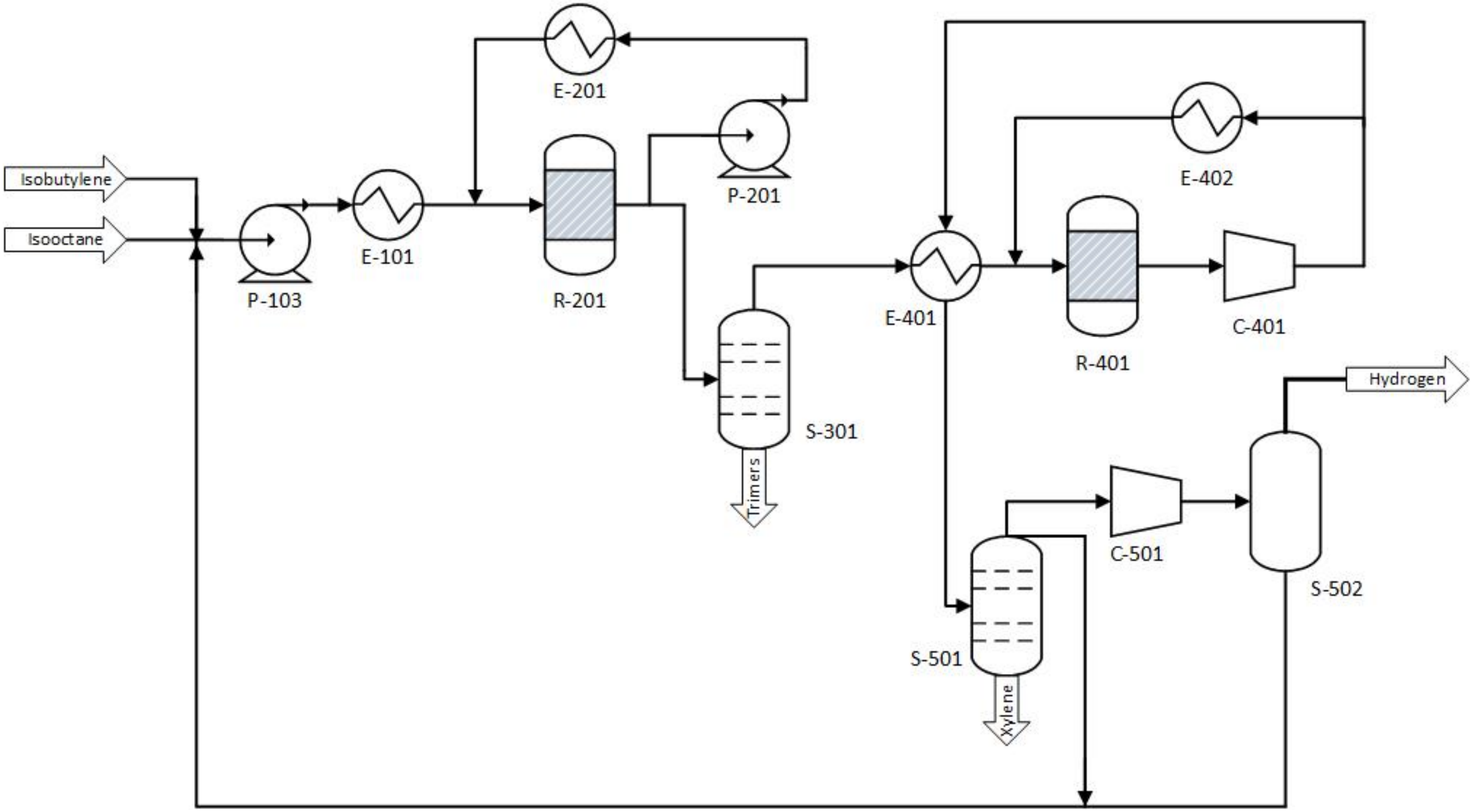
Several catalysts were suggested by the patent to help the oligomerization and dehydrocyclization reactions achieve higher conversions and higher selectivity of the desired product. HZSM-5 was selected for the first reaction while Cr/Al_2O_3 was selected for the second reaction for reasons explained in Section 10.2. Table 11.3 shows properties of the catalysts and their weight hourly space velocity (WHSV) obtained from the patent. WHSV is defined as the mass flow feeding the reactor per catalyst mass, and it indicates how many reactor volumes of feed can be catalyzed in a period of time. Due to the lack of data, the bulk density of Cr/Al_2O_3 was approximated by assuming the mass is mainly attributed to alumina. These properties are then later used to calculate the mass of catalyst in reactors and, subsequently, the volume of the reactors.

Table 11.3 Properties of Catalysts[5] (WHSV = Weight Hourly Space Velocity)

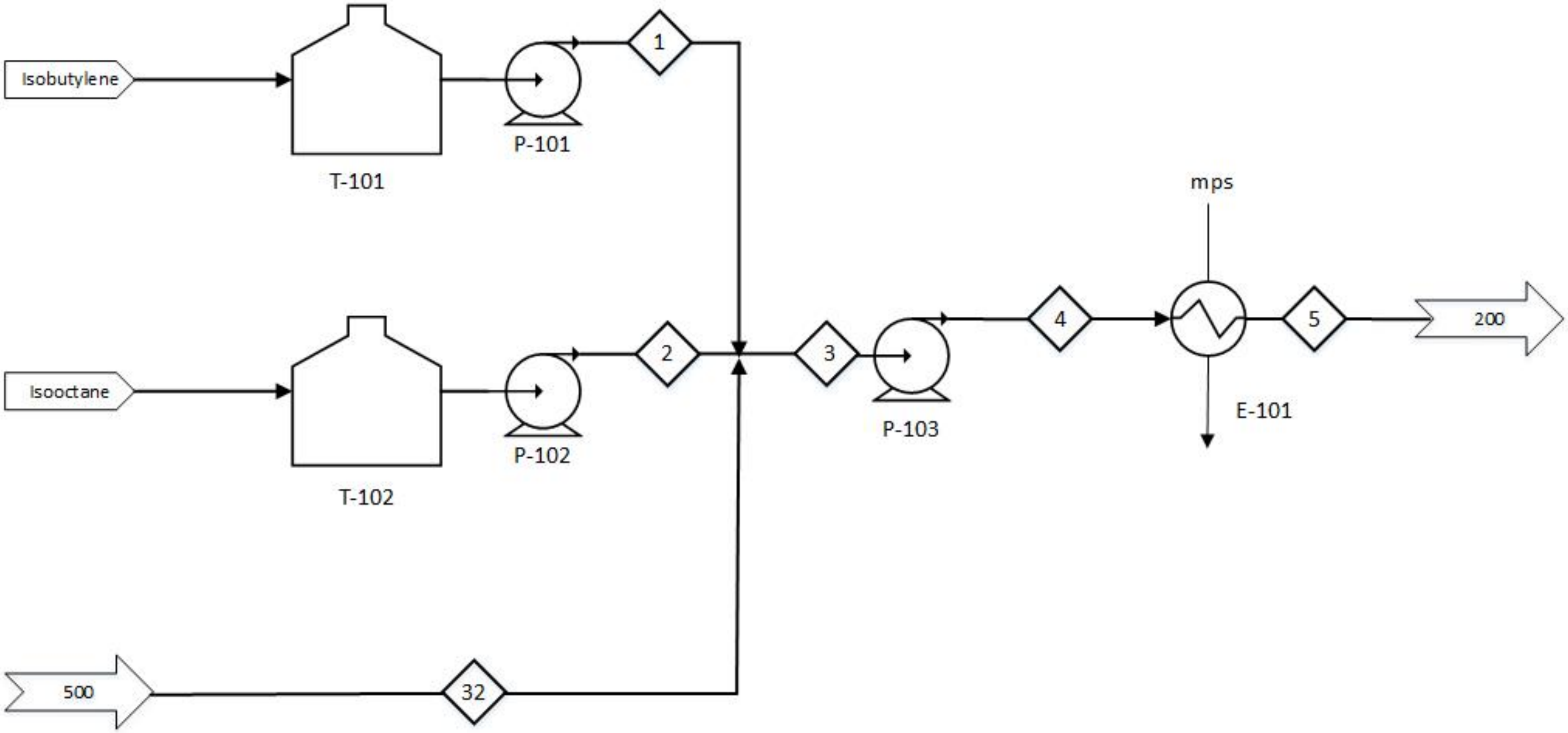
Reaction	**WHSV (hr^{-1})**	**Catalyst**	**Bulk Density (lb/ft^3)**	**Pore Diameter (nm)**	**Important Notes**
Oligomerization	15	HZSM-5	45.26	0.4 – 1.8	-
Dehydrocyclization	1.1	Chromium Oxide Doped Alumina	40.0	6-40	5 % Chromium on Alumina

Section 12
Process Flow Diagram and Material Balances

Overall Flowsheet

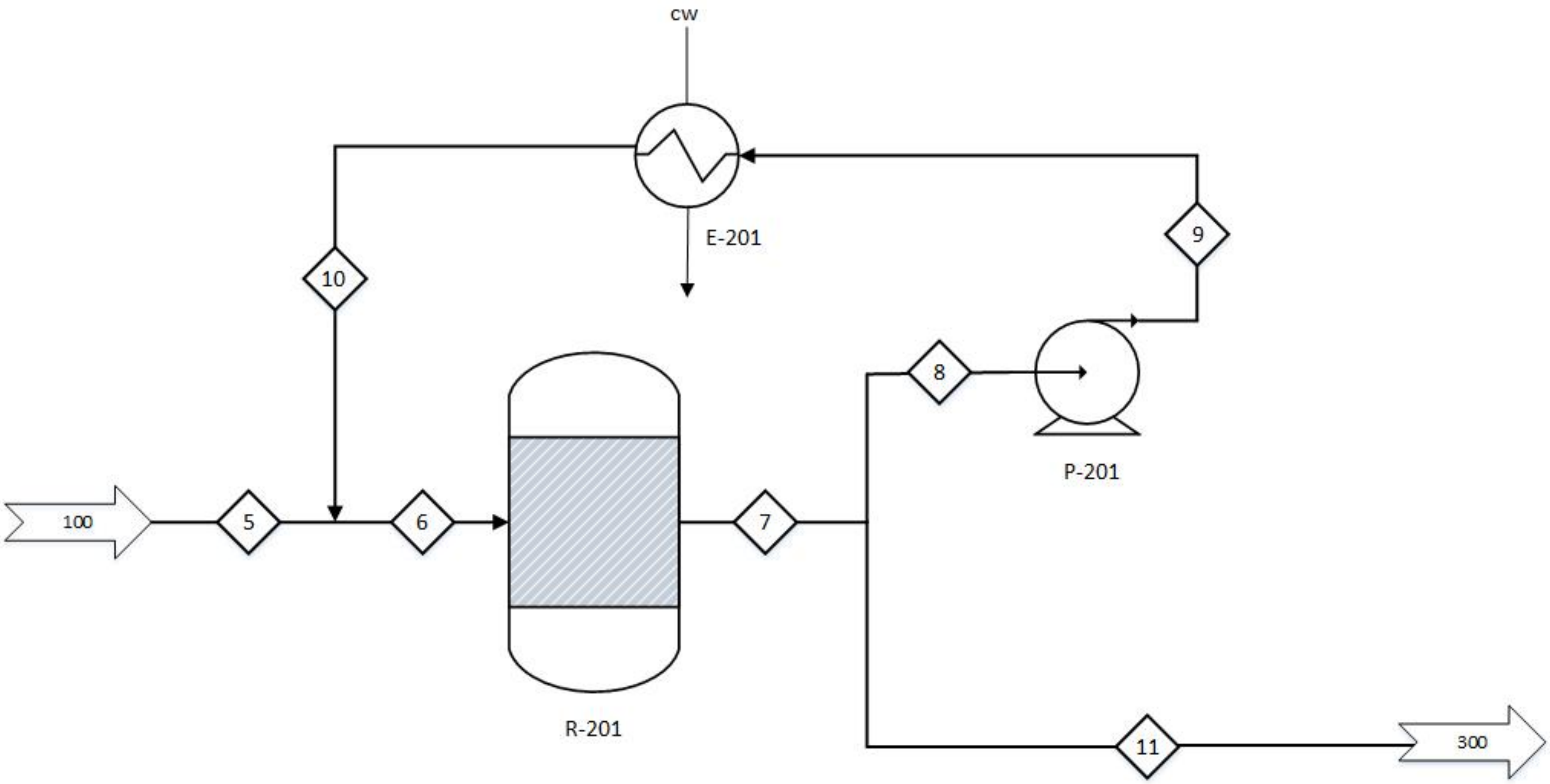


Section 100 - Feed



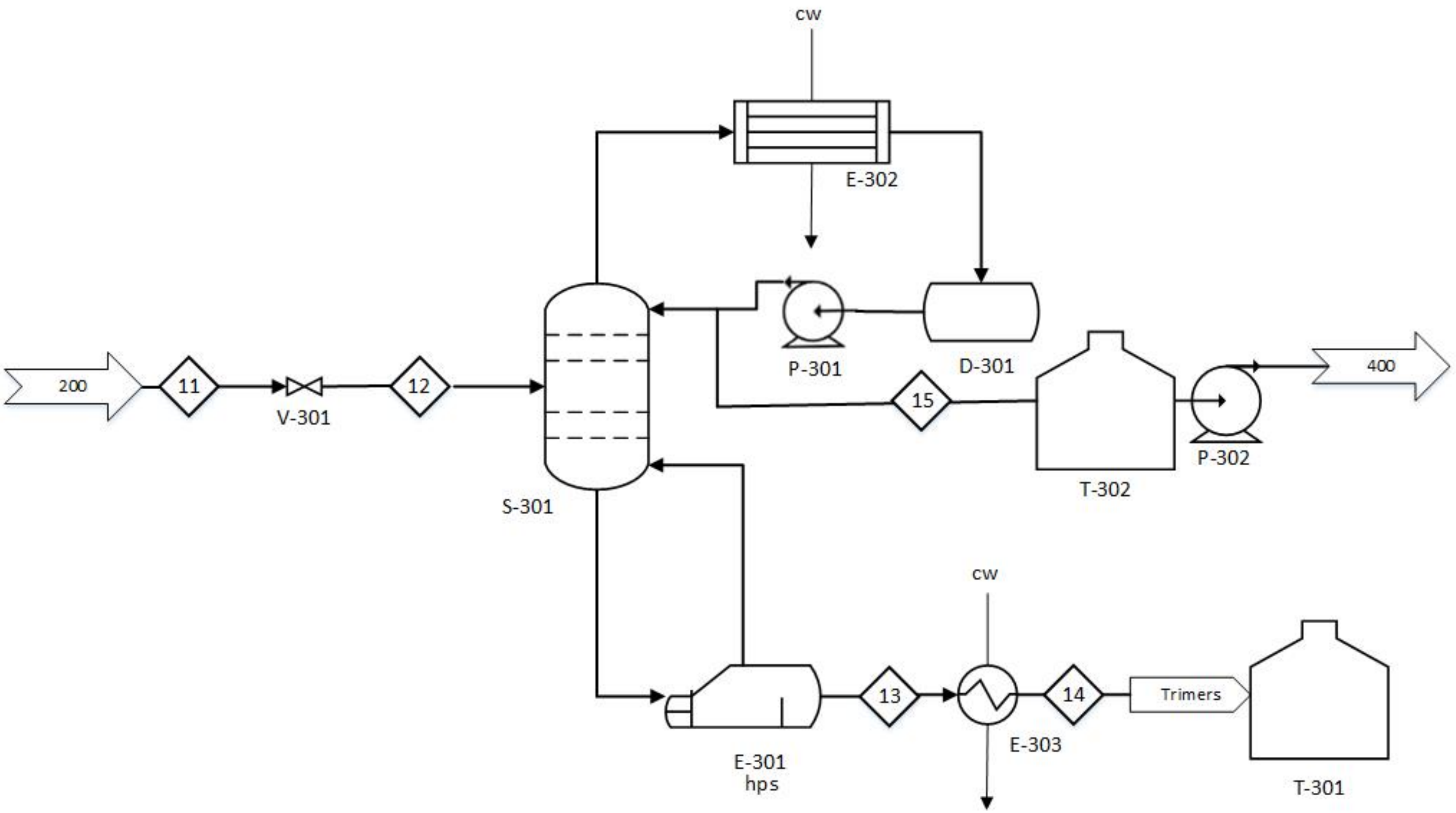
Stream Number	1	2	3	4	5	32
Temperature (°F)	10	80	31	39	347	87
Pressure (psig)	5	0.3	5.3	750	750	15
Vapor fraction	0	0	0	0	0	0
Mass flow (lb/hr)	126820	445.37	181998	181998	181998	54733
Molar flow (lbmol/hr)	2260	4	2755	2755	2755	491
Component Mass Flow (lb/hr)						
Isobutylene	126820	0	127890	127890	127890	1070
para-Xylene	0	0	743	743	743	743
Isooctane	0	445.37	43394	43394	43394	42949
2,4,4-trimethylpentene	0	0	9920.5	9920.5	9920.5	9920.5
Trimers	0	0	0	0	0	0
meta-Xylene	0	0	36	36	36	36
ortho-Xylene	0	0	14	14	14	14
Hydrogen	0	0	0.5	0.5	0.5	0.5

Section 200 – Oligomerization Reactor



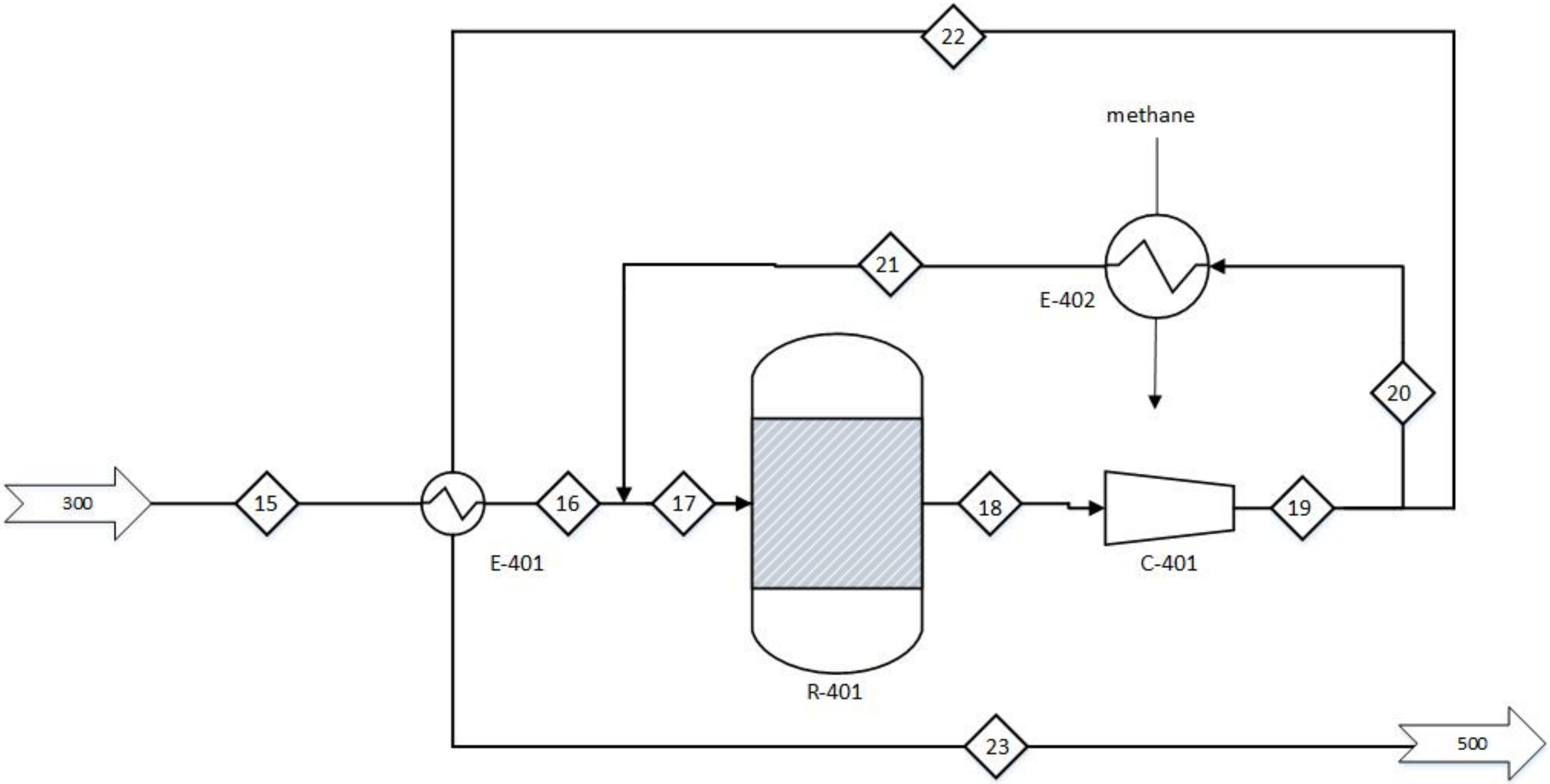
Stream Number	5	6	7	8	9	10	11
Temperature (°F)	347	307	372	372	372	300	372
Pressure (psig)	750	750	750	750	770	770	750
Vapor fraction	0	0	0	0	0	0	0
Mass flow (lb/hr)	181998	1077140	1077140	895140	895104	895140	182000
Molar flow (lbmol/hr)	2755.4	10194	8951	7438	7438	7438	1512
Component Mass Flow (lb/hr)							
Isobutylene	127890	139482	13948	11591	11591	11591	2357
para-Xylene	743	4398	4398	3654	3654	3654	743
Isooctane	43394	256726	256726	213348	213348	213348	43378
2,4,4-trimethylpentene	9920.5	470386	554075	460455	460455	460455	93620
Trimers	0	205849	247694	205842	205842	205842	41851.5
meta-Xylene	36	214	214	178	178	178	36
ortho-Xylene	14	82	82	69	69	69	14
Hydrogen	0.5	3	3	2	2	2	0.5

Section 300 – Trimer Separation



Stream Number	11	12	13	14	15
Temperature (°F)	372	355	543	90	240
Pressure (psig)	750	65	58	45	55
Vapor fraction	0	0	0	0	0
Mass flow (lb/hr)	182000	182000	41852	41852	140148
Molar flow (lbmol/hr)	1512	1512	251	251	1261
Component Mass Flow (lb/hr)					
Isobutylene	2357	2357	0	0	2356
para-Xylene	743	743	56	56	687
Isooctane	43378	43378	209	209	43168.5
2,4,4-trimethylpentene	93620	93620	568	568	93052
Trimers	41851.5	41851.5	41015	41015	837
meta-Xylene	36	36	3	3	33
ortho-Xylene	14	14	2	2	12
Hydrogen	0.5	0.5	0	0	0.5

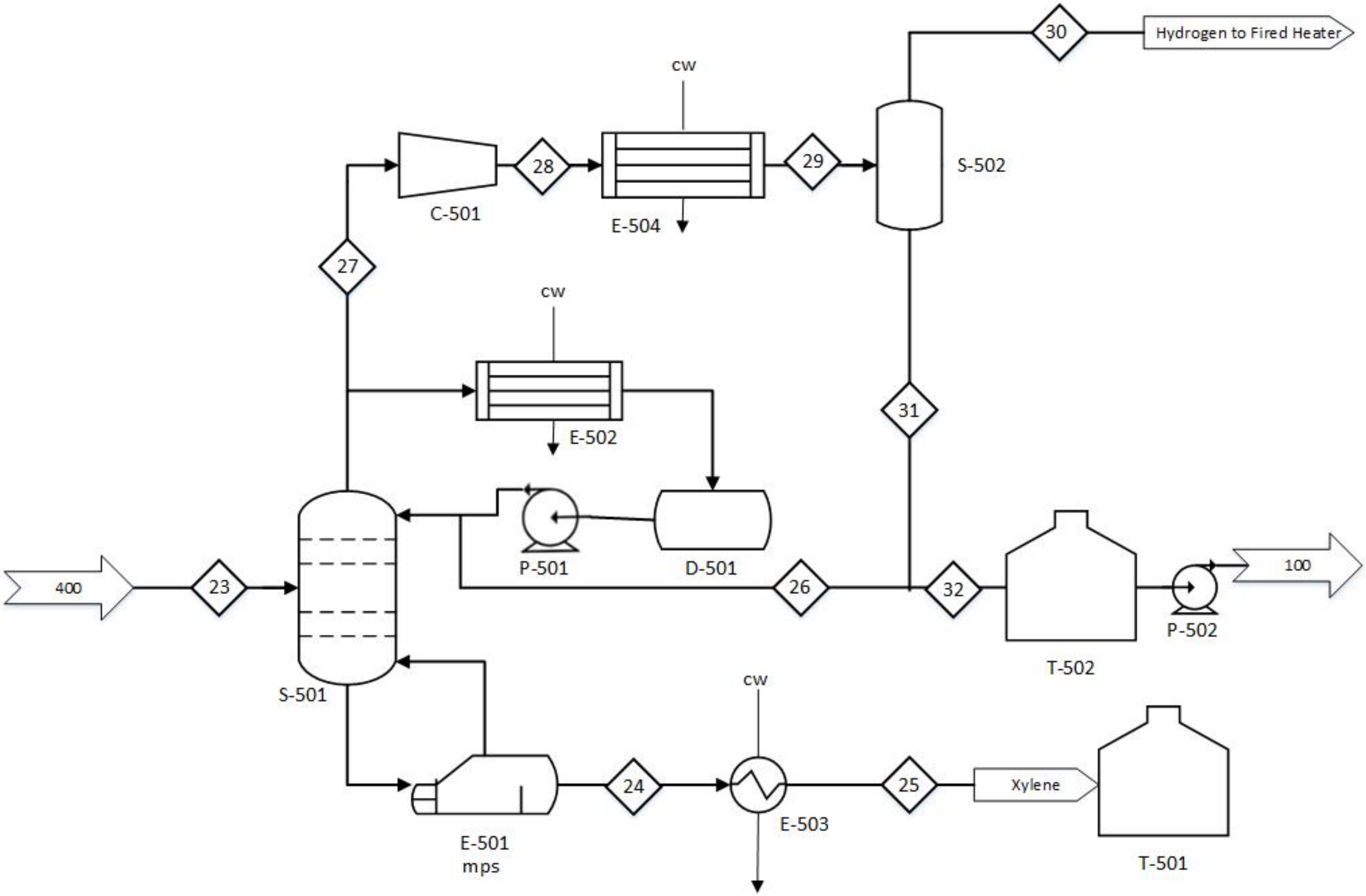
Section 400 – Dehydrocyclization Reactor



Stream Number	15	16	17	18	19	20	21	22
Temperature (°F)	240	856	1034	1001	1022	1022	1050	1022
Pressure (psig)	55	55	30	22	30	30	30	30
Vapor fraction	0	1	1	1	1	1	1	1
Mass flow (lb/hr)	140148	140148	1610150	1610150	1610150	1470000	1470000	140148
Molar flow (lbmol/hr)	1261	1261	37780	40001	40001	36519	36519	3482
Component Mass Flow (lb/hr)								
Isobutylene	2356	2356	27089	27089	27089	24731	24731	2358
para-Xylene	687	687	749675	820401	820401	748993	748993	71408
Isooctane	43168.5	43168.5	496117	496117	496117	452934	452934	43182
2,4,4-trimethylpentene	93052	93052	197763	114702	114702	104719	104719	9984
Trimers	837	837	9625	9625	9625	8787	8787	838
meta-Xylene	33	33	41590	45519	45519	41557	41557	3962
ortho-Xylene	12	12	41336	45265	45265	41325	41325	3940
Hydrogen	0.5	0.5	46955	51431	51431	46954	46954	4477

Stream Number	23		
		Component Mass Flow (lb/hr)	
Temperature (°F)	290		
Pressure (psig)	30	Isobutylene	2358
Vapor fraction	1	para-Xylene	71408
Mass flow (lb/hr)	140148	Isooctane	43182
Molar flow (lbmol/hr)	3482	2,4,4-trimethylpentene	9984
		Trimers	838
		meta-Xylene	3962
		ortho-Xylene	3940
		Hydrogen	4477

Section 500 – Xylene and Hydrogen Separation



Stream Number	23	24	25	26	27	28	29
Temperature (°F)	290	367	90	100	100	454	50
Pressure (psig)	30	30	20	24	24	285	285
Vapor fraction	1	0	0	0	1	1	0.95
Mass flow (lb/hr)	140148	79418	79418	42829.1	17902.6	17902.6	17902.6
Molar flow (lbmol/hr)	3482	745	745	379	2358	2358	2358
Component Mass Flow (lb/hr)							
Isobutylene	2358	0	0	211	2146	2146	2146
para-Xylene	71408	70665	70665	705	38	38	38
Isooctane	43182	38	38	33894	9251	9251	9251
2,4,4-trimethylpentene	9984	25	25	7971	1987	1987	1987
Trimers	838	838	838	0	0	0	0
meta-Xylene	3962	3926	3926	34	2	2	2
ortho-Xylene	3940	3926	3926	13	0.6	0.6	0.6
Hydrogen	4477	0	0	0.1	4476	4476	4476

Stream Number	30	31	32
Temperature (°F)	40	40	87
Pressure (psig)	285	285	24
Vapor fraction	1	0	0
Mass flow (lb/hr)	5997	11904	54733
Molar flow (lbmol/hr)	2245	112	491
Component Mass Flow (lb/hr)			
Isobutylene	1288	859	1070
para-Xylene	0	38	743
Isooctane	196	9055	42949
2,4,4-trimethylpentene	38	1950	9921
Trimers	0	0	0
meta-Xylene	0	2	36
ortho-Xylene	0	1	14
Hydrogen	4476	0.3	0.5

Section 13
Process Description

Section 13.1 Storage Tanks

There will be storage tanks for isobutylene, isooctane, trimers, and xylene. See Section 15 for the design specification of these storage tanks. The raw material storage tanks are discussed here, while the product storage tanks are discussed in Sections 13.3 and 13.5.

Liquid isobutylene is directly pipelined into storage tanks T-101A/B from another plant at our company's site. Isobutylene will enter the process at a flow rate of 126,820 lb/hr. Isobutylene requires two storage tanks due to the large flow rate. This flow rate was calculated by the data given in the problem statement that our company sends our plant 500,000 tons of isobutylene per year and by the industry standard of a 10% downtime. The isobutylene storage tank is designed to contain two-days' worth of isobutylene at 10ºF and 5 psig to prevent a halt in upstream isobutylene production from becoming a bottleneck for this facility. In order to remain liquid at atmospheric pressure, isobutylene must be refrigerated. The refrigeration system on site will be used.

Liquid isooctane, the diluent chosen for this process, is bought from a third-party vendor and stored in the storage tank T-102 at 80ºF and 0.3 psig. To ensure a sufficient amount of diluent is available when starting up the plant initially and that the process will not be halted if the isooctane production is down, a three-week time capacity is chosen. Isooctane exits through the product streams, so 445 lb/hr of isooctane is continuously added to the plant from T-102 to make up for the loss. For start-up, 100,000 lb/hr of isooctane will be added to the system; the tank can manage this amount.

Isobutylene (Stream 1) and isooctane (Stream 2) are pumped out of the storage tanks and mix together with Stream 31, the recycle stream. The resulting flow is at 31ºF and 5.3 psig. While this is the pressure in ASPEN, the mixture should be at higher pressure to avoid flashing. Pump P-103 and heat exchanger E-101 are used to pressurize and heat the stream to 750 psig and 347ºF, the conditions of the oligomerization reactor, R-201. E-101 is a countercurrent heat exchanger that utilizes medium-pressure steam at 150 psig and 366ºF to heat Stream 4.

Section 13.2 Oligomerization Reactor – Section 200

According to the patent, the liquid oligomerization reactions should run at isothermal and isobaric conditions at 347°F and 750 psig. These conditions are achieved using a recirculation stream. Apart from stabilizing reaction conditions, the recirculation stream is also installed for achieving higher overall conversion. Since the reaction is irreversible, sending a portion of the product back to the reactor does not cause equilibrium issues.[10] In combination with the overall recycle stream, this increases the overall conversion of isobutylene in this reactor from 90% to 98%. The portion that proceeds to the rest of the process, Stream 11, is sent to a distillation column to remove trimers before proceeding to R-401, as explained in Section 13.3. The following exothermic reactions are occurring in the reactor to produce both TMP and trimers:

$$2C_4H_8 \rightarrow C_8H_{16}$$

$$3C_4H_8 \rightarrow C_{12}H_{24}$$

Selectivity of dimers is increased by including isooctane as a diluent, as explained in Section 10.1. The ideal composition of the diluent in the reactor feedstock is 20-90%, and in our design, the diluent is about 24% of Stream 6, the inlet to R-201. If further research shows that the percentage of diluent should be higher, this plant can accommodate that change.

Section 13.2.1: Oligomerization Catalyst and Regeneration

The patent gives suggestions on catalyst selection but does not include kinetic data. An HZSM-5 catalyst is used in the fixed bed reactor to selectively produce dimers over trimers. With a WHSV of 15 hr^{-1}, as specified by the patent, the mass of HZSM-5 is 71,809 pounds (see Section 11.4 for catalyst details and the Appendix Section 25.3.3 for catalyst calculations). Decoking will need to occur once every year, and the regeneration time is considered to be 6 hours.[31] Because decoking this reactor would shut down the entire process, decoking can occur during the annual shutdown, so the production rate is not affected. Coke will be burned off by introducing a source of 1% oxygen into the system by the process explained in Section 10.4.[21] After burning, the entire system is flushed with nitrogen to ensure no oxygen remains due to flammability concerns. It is assumed that the catalyst will be fully regenerated by this process, and it will need to be replaced every few years, depending on process data.

Section 13.2.2 R-201 Recirculation Stream

A recirculation loop returns 895,140 lb/hr of the reactor effluent back into the reactor. It is used to improve conversion and mimic isothermal conditions. As stated above, in combination with the overall recycle stream, the recirculation stream improves conversion from 90% to 98%. Before returning to the reactor, Stream 8 is pumped using P-201 and then cooled using the counter-current heat exchanger, E-201, until it reaches 770 psig and 300ºF. E-201 uses cooling water supplied at 86ºF. The formation of both dimers and trimers are exothermic, resulting in an adiabatic temperature rise across the reactor. To mitigate this, Stream 10, the portion recycled back, acts as a heat sink to reduce the adiabatic temperature rise to only 65ºF, a reasonable amount that avoids a runaway reaction. The inlet to the reactor is 40ºF below the reactor condition while the outlet is 25ºF above reactor condition, approximating an isothermal reactor.

Section 13.3 Trimer Separation Column – Section 300

The distillation column, S-301, used to separate the trimers contains 9 theoretical stages, a total condenser, and a kettle reboiler. The feed enters at stage 6, and the condenser pressure is 55 psig. Using ASPEN design specifications, the ideal reflux ratio and bottoms rates to maximize the trimer separation are 0.17 and 41,851 lb/hr, respectively. While the reflux ratio may seem small, some industry processes do have this small ratio.[10] To accommodate the condenser pressure, Stream 11 leaving R-201 is reduced from 750 psig to 65 psig using the valve, V-301. A valve was used instead of a turbine because the stream is liquid, as explained in Section 10.3.

Approximately 98% of the trimers exit as the liquid bottoms product, Stream 13, at 543ºF. About 837 lb/hr of trimers are left in the system. This amount is fairly negligible due to the large size of the other streams; the weight percent of trimers in Stream 15 is only 0.6%. The trimer-rich exit stream can be sold for a financial gain because its composition is similar to kerosene. One disadvantage of operating at these column conditions is that about 800 lb/hr of diluent and TMP is lost through this stream. As mentioned before, the diluent loss is made up by adding isooctane, but the TMP unfortunately cannot be made up. This loss is reasonable because a high trimer separation is achieved. The conditions of this column could be optimized more to reduce the amount of TMP lost and increase the amount of trimers in the exit stream. While we performed as much optimization as possible to achieve an acceptable amount, further analysis could be done. The trimer-rich bottoms will be stored in a storage tank, T-301, which has a time capacity of 2 days.

The remaining TMP in the column comes out as the liquid overhead, Stream 15, at 240ºF and 55 psig and proceeds to the second reactor. To reach the reaction condition of the dehydrocyclization reactor, the liquid overhead is heated by an economizer, E-401, that simultaneously cools the reactor outlet stream. Because each stream has a large temperature difference and one needs to be heated while the other needs to be cooled, pairing the streams reduces the amount of energy needed.

For utilities, the condenser will be using cooling water supplied at 86ºF, and the reboiler will be using high-pressure steam of 1250 psig supplied at 574ºF.

Section 13.4 Dehydrocyclization Reactor – Section 400

Like R-201, the vapor dehydrocyclization reaction should run at isothermal and isobaric condition at 1022ºF and atmospheric pressure as specified by the patent. Industry experts on catalysts say the reactor should not be operated above 30 psig.[10] Again, a recirculation stream is installed to achieve a higher overall conversion and to mimic isothermal conditions. Before the distillate overhead enters the reactor, it mixes with the R-401 recirculation stream to achieve conditions of 1034ºF and 30 psig. This mixed stream, Stream 6, then enters in R-401. Also, as stated previously, the reaction is irreversible so the recycle loop does not cause equilibrium issues.[10] In combination with the overall recycle stream, this increases the 42% conversion of TMP to the three xylene isomers, which was specified by the patent, to 89%. The type of catalyst and diluent can increase the conversion and selectivity of p-xylene, in particular. The same diluent, isooctane, is chosen for this function. The following endothermic reaction is occurring in the reactor to produce the xylene isomers:

$$C_8H_{16} \rightarrow C_8H_{10} + 3H_2$$

The patent specified a weight hourly space velocity of 1.1 hr^{-1}. Following this condition, along with a mass flow rate into the reactor of 536,716 lb/hr, 487,923 pounds of the Cr/Al_2O_3 catalyst is used (see Section 11.4 and 13.4.2 for catalyst details and the Appendix Section 25.3.3

for catalyst calculations). Ideally, a reactor diameter should be no larger than 18 feet for easy transportation and delivery. Due to the size limitation and the massive amount of catalyst required, three reactors are used. They will be set up in parallel because their adiabatic temperature drop of 33ºF is reasonable. This will avoid unnecessary equipment on cooling. The inlet stream will split into three equal streams, each entering a different reactor. It is assumed that the conversion will be split evenly among the three reactors.

A fourth swing reactor will also be in parallel with these reactors. While only three reactors are operating at once, this fourth reactor will undergo the decoking process explained below in Section 13.4.2. This set-up was designed to ease the decoking process and prevent downtime because Cr/Al_2O_3 cokes after five days, so regeneration will need to occur frequently.

Section 13.4.1 R-401 Recirculation Stream

A recirculation loop returns 1.47 MM lb/hr of the reactor effluent back into the reactor. Along with improving the conversion from 42% to 89%, the recirculation loop creates a reasonable adiabatic temperature drop of 33ºF, which is due to the endothermic reactions. The inlet and outlet temperatures are 12ºF above and 21ºF below the specified reaction temperature, approximating an isothermal condition. The outlet of the reactor is still at a very high temperature of 1016ºF, requiring a high-temperature centrifugal blower, C-401, to transport it.

After going through C-401, 1.47 MM lb/hr of the stream is returned to R-401 while the remaining portion continues to the xylene separation column, S-501. To make up for the adiabatic temperature drop, the recycle stream is heated by a fired heater, E-402, to 1050ºF and then mixed with the TMP-rich stream, reaching a temperature and pressure of 1034ºF and 30 psig, respectively.

Section 13.4.2 Decoking of Chromium Oxide Doped Alumina

Regeneration of Cr/Al_2O_3 follows the same procedure as the HZSM-5 catalyst by simply burning off the coke. However, the plant will not stop during the decoking process. Instead, the reactor will be pulled from the process. This is possible because only three reactors need to be operating at one time, and fourth swing reactor will be installed. A valve is controlled to prevent flow into the reactor undergoing the decoking process, while diverting the flow to the recently regenerated reactor. Once another reactor needs to be decoked, the valve to the newly cleaned reactor will open. Once offline, the target reactor will be flushed with a stream that is 1% oxygen to burn off the coke. The entire process will take eight hours, due to the size of the reactors.[21] Reactors can run for five days before they needs to be decoked. The total mass of catalyst in each reactor is 487,923 pounds. Assuming 7% of the catalyst will be covered with carbon, the mass of coke is 34,155 pounds. A stream of 1% oxygen will be burned to decoke the catalyst, which will be initially created from mixing 5 parts of air with 95 parts of nitrogen. For one day of operation with a WHSV of 1.1 hr^{-1}, the coking loss is about 0.3% of reactants fed, which is reasonable.[10] To decrease the amount of nitrogen required, air will be mixed with the gases exiting the decoking process. Approximately 10% of the stream will be purged to get rid of CO_2, and the rest will be recycled back using a blower, as explained in Section 10.4. It is assumed that the catalyst will be fully regenerated by this process, and it will need to be fully replaced every five years. Calculations for catalyst regeneration are in the Appendix, Section 25.3.7.

Section 13.5 p-Xylene Separation – Section 500

A distillation column with 16 theoretical stages, a partial vapor-liquid condenser, and a kettle reboiler are used to separate and purify p-xylene. The feed enters on stage 5, and the condenser pressure is 24 psig. The ASPEN simulation with design specifications on the reflux ratio and bottoms rate yields 1.42 and 79,417 lb/hr, respectively. These are the theoretical ideal conditions for the column to maximize p-xylene purity.

The liquid bottoms product recovers 99% of the inlet p-xylene. The stream is at 367ºF and 30 psig. According to industry consultants, the bottoms temperature should be no higher than 450ºF, so this column is within range. Other xylene isomers, as well as trace amounts of trimers, isobutylene, and isooctane, also leave through this stream, resulting in an 89 wt% p-xylene. This stream is then cooled using a heat exchanger, E-503, before being transported to a third party for further purification.

The condenser produces both a vapor and liquid overhead at 100ºF and 24 psig. Roughly 99.9% of the inlet hydrogen leaves in the condensed vapor product, however, a significant portion of diluent and TMP leaves with hydrogen. The vapor overhead, Stream 27, is pressurized, cooled, and sent to a flash drum. Alternatively, the liquid overhead from the column, Stream 26, is recycled back to the initial feed. The liquid overhead contains 78% of the diluent and 80% of the TMP sent to the column. It is mixed with Stream 31, the liquid bottoms product from the flash, explained in Section 13.6, and recycled as Stream 32. The p-xylene-rich bottom stream from the column will be stored in T-501, which has a time capacity of two days, before being pipelined to the next facility for further purification.

Cooling water supplied at 86ºF is used in the condenser and high-pressure steam of 1250 psig and 574ºF is used in the reboiler to produce the overhead and bottoms products, respectively.

Section 13.6 Diluent Recovery

The vapor overhead from S-501 is fed to a flash to remove hydrogen and recover isooctane. Stream 27 is first fed through a compressor to reach the desired pressure of 285 psig before entering the flash, S-502. The temperature also increases in the compressor to 454ºF. The stream then enters a condenser to decrease the temperature to 50ºF, ensuring a stream of both liquid and vapor enters the flash. The flash, S-502, operates at 40ºF and 285 psig, and it separates the inlet into vapor, Stream 30, and liquid, Stream 31, products. The vapor product contains 99.9% of the inlet hydrogen and 2.2% of the inlet diluent. This vapor product is sent to the fired heater and burned. The remaining 97.8% of the diluent in the liquid bottoms mixes with Stream 26, becoming stream 32, and recycles back to the beginning of the process to mix with the isobutylene feed.

Section 13.7 Surge Tanks

When production halts for decoking or other technical reasons, the material within the system are stored into surge tanks. Two surge tanks are designed for this plant. The first, T-302, is located after S-301 and holds the liquid overhead. The second, T-502, holds the recycle stream. The placement of the first tank serves to decouple the first reactor from the second, so if anything happens upstream, the second reactor can still run using the content of T-302. The second provides the same function but stores the recycle.

Section 14
Energy Balance and Utility Requirements

Section 14.1 Heat Exchanger Network

To minimize the energy input into the plant, as well as decrease the utilities, a heat exchanger network was designed to reuse the energy from the hot streams to heat the cold streams. The network is economically efficient because the design contains several streams that must be heated and several streams that must be cooled. Another reason why this approach works is the range of operating temperatures of the plant.

Specifically, the very high temperature that R-402 operates at requires an inlet stream of 865ºF. In order to do this, very high-pressure steam or a furnace would be required. Handling high-pressure gas in the plant can cause complications and safety hazards. To avoid this, using the outlet of the reactor to heat the inlet was proposed. Therefore, the most notable economizer in this network is E-401, which heats a portion of the reactor feed, Stream 15, with the reactor outlet, Stream 22. The heat duty for this heat-exchanger is 70.9 MM BTU/hr, effectively saving 70.9 MM BTU/hr worth of cooling water and high-pressure steam, shown below in Figure 14.1.

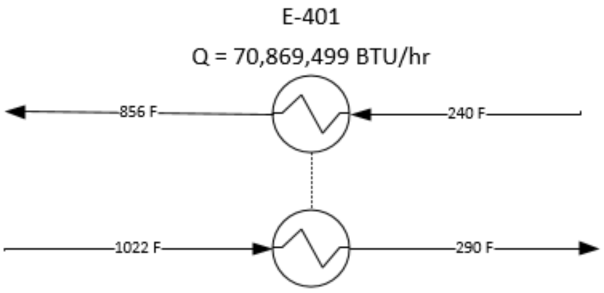


Figure 14.1: Heat Exchanger network for E-401. Stream 15 is heated with Stream 22, and the heat duty is 70.9 MM BTU/hr.

Figure 14.2 shown below illustrates a similar setup for Stream 4 that enters R-201. Because the isobutylene is refrigerated, the feed into R-201 must be heated. Therefore, coupling this with the reactor effluent heat exchanger, which must be cooled due to the adiabatic temperature rise, is possible. Stream 4 can first be heated with Stream 9, resulting in a heat exchanger with 45.9 MM

BTU/hr. After this step of heating, Stream 4 only reaches 324ºF, but it must be at 347ºF to enter the reactor. Therefore, the additional heat can come from cooling the hot xylene stream, Stream 24. This second heat exchanger has a heat duty of 2.30 MM BTU/hr, and it cools the xylene stream to 347ºF. To achieve the 90ºF target temperature for the p-xylene stream, an additional auxiliary heat exchanger is added afterwards utilizing cooling water at 86ºF, resulting in a heat duty of 8.99 MM BTU/hr.

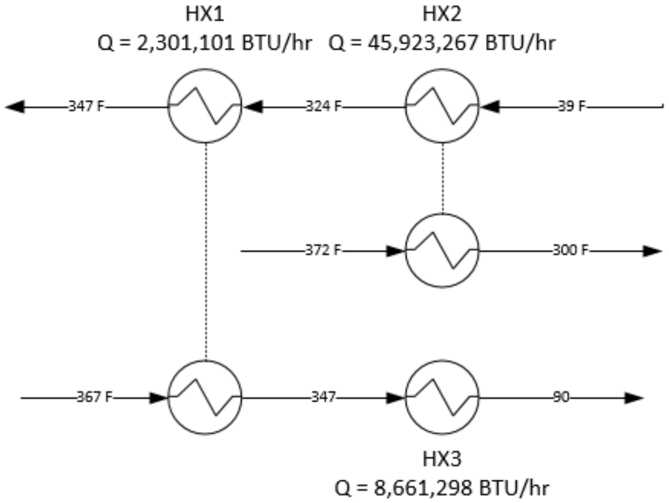


Figure 14.2: Proposed Heat Exchanger Design for Stream 4. Stream 4 would first be heated using Stream 9, resulting in a heat exchanger with a heat duty of 45.9 MM BTU/hr. Then it is heated with the xylene product stream in HX1 to reach the desired 347ºF. An additional auxiliary heat exchanger, HX3, is added to cool the xylene product stream to 90ºF.

Section 14.2 Steam Generation

The numerous hot streams within the network open up the possibility of steam generation. Specifically, the trimer and xylene products, the reboilers for the distillation columns, and the R-201 recirculation loop provide enough energy to convert boiling feed water into steam. The steam generation would decrease the utility cost by removing the need to buy cooling water to cool these streams and removing the need to buy steam to heat other streams. The boiling feed water will enter the heat exchanger at 90 ºF, and the outlet temperature and pressure can be obtained through

ASPEN simulation. The steam can then be sold off for a financial gain or be used in a different section of the plant to heat streams. To optimize costs, steam generation should be utilized.

Section 14.3 Reactor Duty

Reactors are modeled adiabatically in ASPEN; therefore, the corresponding heat duties are zero. In this case, the unreacted reactant, inert species, and product act as a heat source or sink to create an adiabatic temperature rise or drop. The exothermic reactions in R-201 release 15.4 MM BTU/hr. Absorbing this energy causes an adiabatic temperature rise of 65ºF. The endothermic reactions in R-401 require 40.8 MM BTU/hr. Having three reactors allows the needed energy to be shared by all three reactors, causing an adiabatic temperature drop of 33ºF. Both the overall recycle stream and the recirculation streams of each reactor played a part to minimize the temperature change that occurred to mimic isothermal reactors and ensure process safety.

Section 14.4 Fired Heater for R-401 Recirculation Loop

Within the R-401 recirculation loop, the reactor effluent recycles back into the reactor. To make up the temperature loss due to the adiabatic temperature drop, the recycle loop employs a fired heater to increase the temperature from 1022ºF to 1050ºF. A heat exchanger network could not be utilized here due to this being the hottest stream in the process. Additionally, high-pressure steam would not be hot enough. Therefore, a fired heater would need to be used, burning fuel oil to heat the process stream. The fired heater requires 33.3 MM BTU/hr. The trimers have a similar composition to jet fuel, so it was considered to burn the trimers to fuel the fired heater, removing the need to buy fuel from an external source. However, a cost-benefit analysis showed that we would make more money from selling the trimers than we would save from not buying utilities.

As explained in Section 13.6, the hydrogen obtained from the flash drum will be used to fuel the fired heater. This stream is used because it is not pure enough to sell. The hydrogen will only supply 451,000 BTU/hr, which is not enough for the whole fired heater. Looking into other fuel sources, it was found that methane and propane are the most common. Methane is less expensive than propane, so it will be used. To meet the required 33.3 MM BTU/hr of E-401, 1,407 lb/hr of methane gas will be burned in the fired heater.

Section 14.5 Process requirements

Tables 14.1, 14.2, and 14.3 show the hourly and annual utility and electricity requirements for the plant. Pumps and compressors are the main pieces of equipment that consume electricity. Heat exchangers, condensers, and reboilers are the main pieces of equipment that require utilities, such as cooling water, chilled water, and stream. We will use the onsite cooling water tower to treat the circulating cooling water in the process to minimize fouling. Additional utilities include methane, which is burned in the fired heater; nitrogen, which is used to purge the system and during the decoking process; and air, which is also used for the decoking process. For costs, annual usage and costs see Section 19.

Table 14.1 Overall utilities for heat exchangers (Note: B = billion)

	Equipment	Utilities Requirement (BTU/hr)	Quantity (lb/hr)	Quantity (B lb/yr)
Cooling Water	E-201	45,923,300	1,836,975	14.5
	E-302	27,027,281	1,081,117	8.52
	E-303	12,291,800	483,548	3.81
	E-503	11,291,500	451,564	3.56
	E-504A	1,601,657	80,085	0.631
	E-504B	3,140,502	140,000	1.10
	Total	**101,276,040**	**4,073,289**	**32.1**
Chilled Water	E-502	52,041,577	2,081,713	11.9
150 psig Steam	E-101	48,224,368	70,332	0.554
250 psig Steam	E-501	80,409,000	97,347	0.557
1250 psig Steam	E-301	19,167,500	33,219	0.190

Table 14.2 Overall electricity usage for all pumps and compressors

Equipment	hp	kW	Annual kWh
P-101	11	8.2	64,648
P-102	0.05	0.03	265
P-103	378	282	2,222,299
P-201	50	37	293,955
P-301	12	9	70,549
P-302	11	8	64,670
P-501	16	12	94,066
P-502	5	3	26,456
C-401	1	1	5,879
C-501	3,108	2,318	18,272,239
Total	**3,592**	**2,678**	**21,115,026**

Table 14.3 Overall usage of air, nitrogen, and methane

	Purpose	Flowrate (lb/hr)	Flowrate (MM lb/yr)
Air	Decoking	56,924	449
Nitrogen	Purging and Decoking	11,809	93
Methane	Fuel for Fired Heater	1,407	11

Section 15
Equipment List and Unit Description

Section 15.1 Startup

There will be two main differences to acknowledge during startup. First, the flow rates will be larger, so the pumps will need to be able to handle this extra flow. Second, because there are many flammable chemicals in the process, there should be no oxygen present in the process. Therefore, during startup, the system will need to be purged with nitrogen three times. The reactors must also be purged with nitrogen after decoking.

Note: For all costing, earthquakes and wind were not taken into account due to the climate in Iowa.

Section 15.2 Pumps and Compressors

Isobutylene Pump: P-101

Unit ID: P-101	Temperature: 10ºF
Type: Pump	Pressure Change: 5 psig
Material: Carbon Steel	Work: 10.8 hp
Specification Sheet: Section 16, pg. 93	Head: 73 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-101 is a centrifugal pump that pumps isobutylene from the isobutylene storage tanks (T-101A/B) to the process. Because the isobutylene is stored at atmospheric pressure, the pump will need to increase the pressure about 20 psig to send it into the process. Isobutylene needs to enter the process at 126,820 lb/hr. The pump head will be 73 feet, calculated from equations shown in the Appendix, Section 25.3.1. Additionally, the pump will require about 10.8 hp, according to the ASPEN simulation. According to standard guidelines[24], it will be in VSC orientation with 1 stage, a shaft rpm of 3600, and a maximum motor horsepower of 75. The pump efficiency is about 50%, and the calculated power consumption is 10.8 hp. P-101 will be made of carbon steel because isobutylene is not corrosive and will be at ambient temperature. The specification sheet is on page 93. The purchase cost of the pump is $32,000. Because this is a liquid pump, it will have a spare in case of leakage.

Isooctane Pump: P-102

Unit ID: P-102	Temperature: 80 ºF
Type: Pump	Pressure Change: 20 psig
Material: Carbon Steel	Work: 0.05 hp
Specification Sheet: Section 16, pg. 94	Head: 69 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-102 is a centrifugal pump that pumps isooctane from the isooctane storage tank (T-102) to the process. Because the isooctane is stored at atmospheric pressure, the pump will need to increase the pressure about 20 psig to send it into the process. Isooctane needs to enter the process at 445 lb/hr to make up for the amount leaving the process through the three exit streams. The pump head will be 69 feet, calculated from equations shown in the Appendix, Section 25.3. Additionally, the pump will only require about 0.05 hp, according to the ASPEN simulation. The horsepower is small due to the low flow rate. According to standard guidelines[24], it will be in VSC orientation with 1 stage, a shaft rpm of 3600, and a maximum motor horsepower of 75. The pump efficiency is about 50%, and the calculated power consumption is 0.05 hp. P-102 will be made of carbon steel because isooctane is not corrosive and will be at ambient temperature. The specification sheet is on page 94. The purchase cost of the pump is $32,000. Because this is a liquid pump, it will have a spare in case of leakage. For startup, 100,000 pounds of isooctane will need to be added to inventory the process. P-201 can handle this amount.

R-201 Feed Pump: P-103

Unit ID: P-103	Temperature: 31 ºF
Type: Pump	Pressure Change: 745 psig
Material: Carbon Steel	Work: 337 hp
Specification Sheet: Section 16, pg. 95	Head: 2,750 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-103 is a centrifugal pump that increases the pressure of the mixture of pure isobutylene, pure isooctane, and the recycle loop to match the pressure of R-201. The mixture is at about atmospheric pressure and needs to increase to slightly above 750 psig. 181,998 lb/hr of the mixture is flowing through the pump. Therefore, the pump head will be 2,750 feet, calculated from equations shown in the Appendix, Section 25.3.1. Additionally, the pump will require about 337 hp of work, according to the ASPEN simulation. According to standard guidelines[24], it will be in HSC orientation with 2, or possibly more, stages, a shaft rpm of 3600, and a maximum motor horsepower of 1450. The pump efficiency is about 73%, and the calculated power consumption is 378 hp. These calculations are also shown in the Appendix, Section 25.3.1. P-103 will be made of carbon steel because the chemicals are not corrosive and the temperature is fairly low. The specification sheet is on page 95. The purchase cost of the pump is $189,900. Because this is a liquid pump, it will have a spare in case of leakage.

R-201 Recirculation Pump: P-201

Unit ID: P-201	Temperature: 373 ºF
Type: Pump	Pressure Change: 20 psig
Material: Carbon Steel	Work: 47 hp
Specification Sheet: Section 16, pg. 96	Head: 84 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-201 is a centrifugal pump that pumps 895,140 lb/hr of the process fluid through the R-201 recirculation loop. The pump head will be 84 feet, calculated from equations shown in the Appendix, Section 25.3.1. Additionally, the pump will require about 47 hp, according to the ASPEN simulation. According to standard guidelines[24], it will be in HSC orientation with 1 stage, a shaft rpm of 1800, and a maximum motor horsepower of 250. The pump efficiency is about 84%, and the calculated power consumption is 50 hp. P-201 will be made of carbon steel because the chemicals are not corrosive and the temperature is reasonable. The specification sheet is on page 96. The purchase cost of the pump is $41,800. Because this is a liquid pump, it will have a spare in case of leakage.

T-302 Pump: P-302

Unit ID: P-302	Temperature: 240 ºF
Type: Pump	Pressure Change: 55 psig
Material: Carbon Steel	Work: 11 hp
Specification Sheet: Section 16, pg. 117	Head: 96 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-302 is a centrifugal pump that increases the pressure of the process stream after it has been stored in the surge tank. The mixture is at atmospheric pressure and needs to increase to 55 psig. 140,148 lb/hr of the mixture is flowing through the pump. Therefore, the pump head will be 96 feet, calculated from equations shown in Appendix, Section 25.3.1. Additionally, the pump will require about 11 hp, according to the ASPEN simulation. According to standard guidelines[24], it will be in VSC orientation with 1 stage, a shaft rpm of 3600, and a maximum motor horsepower of 75. The pump efficiency is about 70%, and the calculated power consumption is 11 hp. P-302 will be made of carbon steel because the chemicals are not corrosive and the temperature is fairly low. The specification sheet is on page 117. The purchase cost of the pump is $6,800. Because this is a liquid pump, it will have a spare in case of leakage.

T-502 Pump: P-502

Unit ID: P-302	Temperature: 87 ºF
Type: Pump	Pressure Change: 24 psig
Material: Carbon Steel	Work: 4 hp
Specification Sheet: Section 16, pg. 119	Head: 80 ft
Costing Data: Section 17	Design Calculation: Section 25.3.1

P-502 is a centrifugal pump that increases the pressure of the recycle stream after it has been stored in the surge tank. The mixture is at atmospheric pressure and needs to increase to about 24 psig to enter the process again. 54,733 lb/hr of the mixture is flowing through the pump. Therefore, the pump head will be 80 feet, calculated from equations shown in Appendix, Section 25.3.1. Additionally, the pump will require about 4 hp, according to the ASPEN simulation. According to standard guidelines[24], it will be in VSC orientation with 1 stage, a shaft rpm of 3600, and a maximum motor horsepower of 75. The pump efficiency is about 59%, and the calculated power consumption is 4 hp. P-502 will be made of carbon steel because the chemicals are not corrosive and the temperature is fairly low. The specification sheet is on page 119. The purchase cost of the pump is $8,600. Because this is a liquid pump, it will have a spare in case of leakage.

R-401 Recirculation Blower: C-401

Unit ID: C-401	Temperature: 1,020 ºF
Type: Centrifugal Turbo Blower	Pressure Change: 22 psig
Material: Stainless Steel	Work: 11,009 hp
Specification Sheet: Section 16, pg. 97	Design Calculation: Section 25.3.1
Costing Data: Section 17	

C-401 is a centrifugal blower used in the R-401 recirculation loop. Due to the very high temperature of the process vapor going through the compressor of 1,000 ºF, the compressor will need to be made of Stainless Steel, which can withstand 1,300ºF. The pressure of the vapor entering the compressor is low at 22 psig, and the flow rate is 1,610,150 lb/hr. To increase the pressure to 30 psig, the blower will require 11,009 hp. A low pressure change means a low compression ratio, so multiple stages are not needed. The purchase cost of the blower is $5,498,000. This high cost was expected due to the large flow rate and expensive material of construction. The specification sheet is on page 97.

S-502 Compressor: C-501 (E-503A/B)

Unit ID: C-501	Temperature: 454 ºF
Type: Multi-Stage Compressor	Pressure Change: 260 psig
Material: Carbon Steel	Work: 3,207 hp
Specification Sheet: Section 16, pg. 98	# of Stages: 3
Costing Data: Section 17	Design Calculation: Section 25.3.1

C-501 is a centrifugal compressor used to increase the pressure of the vapor stream out of S-501 to 285 psig to match the conditions needed for S-502 to recover hydrogen. The vapor stream is 17,903 lb/hr and 100ºF. The compressor is isentropic with an efficiency of 85%. If one compressor were to be used, the compression ratio would be about 12. According to common practice, each stage can only handle a compression ratio of about 3. Because of the large increase in pressure, the temperature increases as well. To avoid damaging the compressor, there will need to be multiple stages with intercoolers (using cooling water) in between. The first stage will increase the pressure from 24 psig to 70 psig, requiring 1038 hp and increasing the temperature 124ºF. The intercooler will mostly maintain the pressure, except for an assumed 5 psig pressure drop, and decrease the temperature to 150ºF. The second stage will increase the pressure to 200 psig, requiring 1526 hp. This will cause an increase in temperature of 190ºF, so the next intercooler will decrease the temperature to 200ºF. The third and final stage will increase the pressure to the desired amount of 285 psig, requiring 643 hp. It will be an electric compressor made of carbon steel because there is no corrosion and the temperature is within the specifications. The three stages will require a total of 3,207 hp. The specification sheet is on page 98. The purchase cost of the compressor is $1,961,000.

The first intercooler will have an area of 170 ft^2. It will be used to cool the process stream from 224ºF to 150ºF. This will require 1041 hp, and 80,085 lb/hr of cooling water will be used. The second intercooler will have an area of 170 ft^2. It will be used to cool the process stream from 340ºF to 200ºF. This will require 1234 hp, and 140,000 lb/hr of cooling water will be used. The costs of the intercoolers are $12,100 and $12,500. Calculations are shown in the Appendix, Section 25.3.2.

Section 15.3 Heat Exchangers

It is assumed that there will be a 10 psig pressure drop across all heat exchangers. In this list, heat exchangers use cooling water and steam to cool and heat the process streams, respectively; however, some of the utilities can be removed by building the heat exchanger network that was described in Section 14.1.

R-201 Feed Heat Exchanger: E-101

Unit ID: E-101	Temperature Change: 308 ºF
Type: Counter-Current Heat Exchanger	Pressure: 750 psig
Material: Carbon Steel	Area: 2,977 ft^2
Specification Sheet: Section 16, pg. 101	Heat Duty: 48,224,400 BTU/hr
Costing Data: Section 17	Design Calculation: Section 25.3.2

E-101 is used to heat the mixture of pure isobutylene, pure isooctane, and the recycle loop to the temperature of R-201. The temperature is initially at 39 ºF and needs to be increased to 347ºF, so medium-pressure steam of 150 psig will be used. The process fluid enters the tube at 181,998 lb/hr. According to ASPEN, the heat exchanger has a heat duty of 48.2 MM BTU/hr.

Using the heat of vaporization and the heat duty, 40,3210 lb/hr of steam will be used. The heat transfer coefficient is 150 BTU/(ºF*ft^2*hr), obtained from standard guidelines[24]. Rigorous calculations using these variables are shown in Appendix, Section 25.3.2 according to standard equations[24]. The log-mean-temperature-difference (LMTD) is 108ºF, making the area of the heat exchanger 2,977 ft^2. Assuming a tube velocity of 3 ft/s and an inner tube diameter of 1 inch, there will need to be 78 tubes of length 24 ft. The number of passes per tube will need to be 6. The shell diameter is 37 inches. Both the shell and tube will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 101. The purchase cost of the heat exchanger is $42,900.

R-201 Recirculation Heat Exchanger: E-201

Unit ID: E-201	Temperature Change: 72 ºF
Type: Counter-Current Heat Exchanger	Pressure: 785 psig
Material: Carbon Steel	Area: 1,892 ft^2
Specification Sheet: Section 16, pg. 102	Heat Duty: 45,923,300 BTU/hr
Costing Data: Section 17	Design Calculation: Section 25.3.2

E-201 is used to cool the process fluid in the recirculation loop around R-201 due to the adiabatic temperature rise in the reactor from the exothermic reaction. The temperature of the fluid enters E-201 at 372 ºF and is cooled to 300 ºF using cooling water. The process fluid enters the shell at 895,140 lb/hr. According to ASPEN, the heat exchanger has a heat duty of 45.9 MM BTU/hr. Assuming that the cooling water will enter the tube at 86ºF and increase 25ºF, the mass flow rate of the cooling water was calculated to be 1,836,975 lb/hr. The heat transfer coefficient is 100 BTU/(ºF*ft^2*hr), obtained from standard guidelines.[24] Rigorous calculations using these variables are shown in the Appendix, Section 25.3.2 according standard equations.[24] The LMTD is 243ºF, making the area of the heat exchanger 1,892 ft^2. Assuming a tube velocity of 8 ft/s and an inner tube diameter of 1 inch, there will need to be 189 tubes of length 24 ft. The number of passes per tube will need to be 2. Therefore, using standard data and assuming a square pitch, the shell inner diameter is 31 inches.[24] Both the shell and tube will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 102. The purchase cost of the heat exchanger is $33,200.

Trimer Stream Heat Exchanger: E-303

Unit ID: E-303	Temperature Change: 453 ºF
Type: Counter-Current Heat Exchanger	Pressure: 55 psig
Material: Carbon Steel	Area: 1,085 ft^2
Specification Sheet: Section 16, pg. 103	Heat Duty: 12,291,800 BTU/hr
Costing Data: Section 17	Design Calculation: Section 25.3.2

E-303 is used to cool the bottom stream exiting S-301, which is mainly trimers. Trimers can be stored at ambient temperature, so the heat duty from the heat exchanger can be used somewhere else in the process. The temperature of the fluid enters E-303 at 543ºF and is cooled to 90ºF using cooling water. The process fluid enters the shell at 41,852 lb/hr. According to ASPEN, the heat exchanger has a heat duty of 12.3 MM BTU/hr. Assuming that the cooling water will enter the tube at 86ºF and increase 25ºF, the mass flow rate of the cooling water was calculated to be 483,548 lb/hr. The heat transfer coefficient is 100 BTU/(ºF*ft^2*hr). Rigorous calculations using these variables are shown in the Appendix, Section 25.3.2 according to standard equations.[24] The LMTD is 113ºF, making the area of the heat exchanger 1,085 ft^2. Assuming a tube velocity of 5 ft/s and an inner tube diameter of 1 inch, there will need to be 80 tubes of length 24 ft. The number of passes per tube will need to be 2. Therefore, using standard guidelines[24] and assuming a square pitch, the shell inner diameter is 21¼ inches. Both the shell and tube will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 103. The purchase cost of the heat exchanger is $22,100.

R-401 Feed Heat Exchanger: E-401

Unit ID: E-401	Temperature Change: 641 ºF (tube), 756 ºF (shell)
Type: Counter-Current Heat Exchanger	Pressure: 43 psig
Material: Stainless Steel	Area: 16,350 ft^2
Specification Sheet: Section 16, pg. 104	Heat Duty: 70,869,600 BTU/hr
Costing Data: Section 17	Design Calculation: Section 25.3.2

E-401 is a counter-current heat exchanger using process fluids in both the tubes and shell. The fluid coming from S-301 and going to R-401 will need to be heated to meet the high temperature condition of R-401. The stream leaving R-401 and going to S-501 will be cooled from its high temperature to the conditions of S-501. An economizer is used here so that the hot stream heats the cold stream, without the need of other utilities. The 140,148 lb/hr cold stream, coming from the separation column, enters the heat exchanger at 240ºF and leaves at 881ºF. The 140,148 lb/hr hot stream, coming from the reactor, enters the heat exchanger at 1,046ºF and exits at 290ºF. According to ASPEN, the heat exchanger has a heat duty of 70.9 MM BTU/hr. The heat transfer coefficient is 45 BTU/(ºF*ft^2*hr), according to standard guidelines.[24] Rigorous calculations using these variables are shown in the Appendix, Section 25.3.2 according to standard equations.[24] The LMTD is 96ºF, making the area of the heat exchanger 16,350 ft^2. Assuming a tube velocity of 2 ft/s and an inner tube diameter of 1 inch, there will need to be 92 tubes of length 30 ft. The number of passes per tube will need to be 23. This is too large, so other configurations should be considered, such as 2 heat exchangers. To decrease the number of tubes per pass, the LMTD must be greater. Both the shell and tube will be made of stainless steel because although the fluid is non-corrosive, the high temperature requires a stronger material. The specification sheet is on page 104. The purchase cost of the heat exchanger is $586,300.

Xylene Stream Heat Exchanger: E-503

Unit ID: E-503	Temperature Change: 287 ºF
Type: Counter-Current Heat Exchanger	Pressure: 30 psig
Material: Carbon Steel	Area: 1,467 ft^2
Specification Sheet: Section 16, pg. 105	Heat Duty: 11,291,500 BTU/hr
Costing Data: Section 17	Design Calculation: Section 25.3.2

E-503 is used to cool the bottom stream exiting S-501, which is mainly the desired product, xylene. Xylene can be stored at ambient temperature, so the heat duty from the heat exchanger can be used somewhere else in the process. The temperature of the fluid enters E-503 at 366ºF and is cooled to 90ºF using cooling water. The process fluid enters the shell at 79,418 lb/hr. According to ASPEN, the heat exchanger has a heat duty of 11.3 MM BTU/hr. Assuming that the cooling water will enter the tube at 86ºF and increase 25ºF, the mass flow rate of the cooling water was calculated to be 451,564 lb/hr. The heat transfer coefficient is 100 BTU/(ºF*ft^2*hr). Rigorous calculations using these variables are shown in the Appendix, Section 25.3.2 according to standard equations.[24] The LMTD is 77ºF, making the area of the heat exchanger 1,467 ft^2. Assuming a tube velocity of 5 ft/s and an inner tube diameter of 1 inch, there will need to be 75 tubes of length 24 ft. The number of passes per tube will need to be 4. Therefore, using standard guidelines[24] and assuming a square pitch, the shell inner diameter is 31 inches. Both the shell and tube will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 105. The purchase cost of the heat exchanger is $26,200.

R-401 Recirculation Fired heater: E-402

Unit ID: E-402	Temperature Change: 28 ºF
Type: Fired heater	Pressure: 30 psig
Material: Cr-Mo Alloy Steel	Heat Duty: 33,355,300 BTU/hr
Specification Sheet: Section 16, pg. 106	Costing Data: Section 17

E-402 is used to heat the process fluid in the recirculation loop around R-401 due to the adiabatic temperature drop in the reactor from the endothermic reaction. The process vapor enters the heat exchanger at 1022ºF and is heated to 1050ºF. It has a flow rate of 1,470,000 lb/hr. According to ASPEN, the heat exchanger has a heat duty of 13,109 hp. The fired heater is made out of Cr-Mo Alloy Steel because the fluid is non-corrosive and this option was the cheapest. The specification sheet is on page 106. The purchase cost of the heat exchanger is $1,084,000.

Section 15.4 Reactors

Oligomerization Reactor: R-201

Unit ID: R-201	Temperature: 240 ºF
Type: Reactor	Pressure: 750 psig
Material: Carbon Steel	Volume: 1,745 ft^3
Specification Sheet: Section 16, pg. 107	Heat Duty: 0 BTU/hr (adiabatic)
Costing Data: Section 17	Diameter: 8 ft
Design Calculation: Section 25.3.3	Height: 33 ft

R-201 is a packed bed reactor. The desired reaction in R-201 converts liquid isobutylene into liquid TMP. The undesired reaction creates liquid trimers. The reactor conditions are 340ºF and 750 psig. Due to a large recirculation loop, 1,077,140 lb/hr enter the reactor. The reaction is exothermic with a reasonable adiabatic temperature rise of 65ºF. The patent gives a weight hourly space velocity (WHSV) of 15 hr^{-1}. Using the WHSV, the volumetric flowrate, and the bulk density of the HZSM-5 catalyst, which is 45 lb/ft^3, the mass of the catalyst was calculated to be 71,809 lbs, with a volume of 1,587 ft^3.[5] Assuming the volume of the catalyst is equal to the volume of the reactor, and adding in a 10% safety factor, the volume of the reactor is 1,745 ft^3. This gives a residence time of 3.44 min. Assuming an L/D ratio of 4, the diameter is 8 ft and the height is 33 ft. The superficial fluid velocity is 0.16 ft/s, which is similar to other liquid reactions. These calculations are also shown in the Appendix, Section 25.3.3. The reactor will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 107. The purchase cost of the reactor is $384,400.

Dehydrocyclization Reactors: R-401, R-402, R-403, and R-404

Unit ID: R-401,2,3,4	Temperature: 1028 ºF
Type: Reactor	Pressure: 22 psig
Material: Stainless Steel	Volume/Reactor: 13,411 ft^3
Specification Sheet: Section 16, pg. 108	Heat Duty: 0 BTU/hr (adiabatic)
Costing Data: Section 17	Diameter/Reactor: 16 ft
Design Calculation: Section 25.3.3	Height/Reactor: 65 ft

R-401 is a packed bed reactor. The desired reaction in R-401 converts vapor TMP into vapor p-xylene. The undesired reactions create vapor m- and o-xylene. The reactor conditions are 1028ºF and 22 psig. Due to a large recirculation loop, 1,610,148 lb/hr enter the reactor. Because of the large flow rate, which would also mean a large volume of catalyst, there will actually be three reactors instead of one. This also allows the L/D ratio to remain at 4. This means that 536,716 lb/hr will enter each of the reactors. It is assumed that each reactor will do one third of the total overall conversion, so each reactor will be identical. The reaction is endothermic with a reasonable adiabatic temperature drop of 33ºF. The reactors will be in parallel, so only the feed into the reactor needs to be heated, and heating does not have to occur between each reactor. The patent gives a WHSV or 1.1 hr^{-1}. Using the WHSV, the volumetric flowrate, and the bulk density of the chromium oxide doped alumina catalyst, which is 40 lb/ft^3, the mass of the catalyst per reactor was calculated to be 487,924 lbs, with a volume of 12,192 ft^3.[5] Assuming the volume of the catalyst is equal to the volume of the reactor, and adding in a 10% safety factor, the volume of the reactor is 13,411 ft^3. This gives a residence time of 0.16 min per reactor. Assuming an L/D ratio of 4, the diameter is 16 ft and the height is 65 ft. The superficial fluid velocity is 6.92 ft/s, which is similar to other vapor reactions. Because the catalyst cokes and must be regenerated every fifth day, there will be a swing reactor, meaning there will be four reactors in parallel. Three reactors will always be operating, then when one needs to be regenerated, it will be taken offline and the one that was just regenerated will be placed into the process (by opening and closing valves). The swinging design allows for less downtime. It is assumed that the catalyst will need to be replaced every 5 years. These calculations are also shown in the Appendix, Section 25.3.3. The reactor will be made of stainless steel because even though the fluid is non-corrosive, the operating temperature is very high. The specification sheet is on page 108. The purchase cost of each reactor is $384,400.

Section 15.5 Distillation Columns and Flash Drum

Trimer Separation Distillation Column: S-301 (D-301, E-301, E-302, P-301)

Unit ID: S-301	Temperature: 355 ºF
Type: Distillation Column	Pressure: 65 psig
Material: Carbon Steel	Diameter: 9 ft
Specification Sheet: Section 16, pg. 109	Height: 44 ft
Costing Data: Section 17	Design Calculation: Section 25.3.4

The function of S-301 is to remove the undesirable trimers from the process. A liquid stream, mostly containing TMP, isooctane, and trimers, enters the column at 182,000 lb/hr, and the two exit streams leave the column as liquids. In the ASPEN simulation, this separation requires 9 stages, a feed at stage 6, a condenser pressure of 84 psig, a condenser pressure drop of 0.2 psig, a stage pressure drop of 0.12 psig, a reflux ratio of 0.17, and a bottoms flow rate of 41,852 lb/hr. ASPEN was used to obtain the height and diameter measurements of the column. With only one pass over the trays, the diameter is 9 feet, which is very reasonable. This number of trays was used to calculate the height. It is industry standard to have 2 feet of spacing between each tray. Additionally, a sump space of 4 feet was added, a headspace of 10 feet, a disengaging space of 3 feet, and a feed location spacing of 3 feet, were factored in. While ASPEN gives the theoretical number of stages, the actual number of trays was calculated through the O'Connell Correlation, which takes the efficiencies of the trays into account. This correlation indicates that there should be 17 trays, with a feed on tray 11, and a tray efficiency of 0.44. Therefore, the height of the column is 44 feet. This creates an L/D ratio of about 5. The total pressure drop over the column, calculated from ASPEN, is 0.7 psig. These calculations are also shown in the Appendix, Section 25.3.4. All parts of the column will be made out of carbon steel, again because the process fluid is non-corrosive and the temperature is within range of the material. The specification sheet is on page 109. The purchase cost of the column is $150,015.

The reflux accumulator, D-301, was designed as a horizontal pressure vessel. It was assumed that it would have a residence time of 5 min and an L/D ratio of 2. Using a flow of 163,277 lb/hr, the reflux accumulator will have a diameter of 8 ft and a height of 15 ft. The purchase cost of the reflux accumulator is $36,269.

The reflux pump, P-301, has a head of 93 ft, an isentropic efficiency of 0.718, and requires 12 hp. This was calculated by assuming a pressure drop of 20 psig and using equations in the Appendix, Section 25.3.1. The purchase cost of the reflux pump is $8,969, which will have a spare.

The total condenser will be maintained at 240ºF by using 1,081,117 lb/hr of cooling water. According to ASPEN, the condenser has a heat duty of 27.0 MM BTU/hr. The heat transfer coefficient is 100 BTU/(ºF*ft^2*hr). Using the calculations in the Appendix, Section 25.3.2, the area of the condenser is 1,837 ft^2. Assuming a tube velocity of 5 ft/sec, there will be 178 tubes with 2 passes per tube, 20 ft long tubes, and an inner shell diameter of 37 inches. The purchase cost of the condenser is $26,771.

The reboiler will be maintained at 543ºF by using very high-pressure steam of 1250 psig. According to ASPEN, the reboiler has a heat duty of 19,167,500 BTU/hr. The heat transfer coefficient is 150 BTU/(ºF*ft^2*hr). Using the calculations in the Appendix, Section 25.3.2, the area of the reboiler is 42,594 ft^2. Assuming a tube velocity of 2 ft/sec, there will be 33 tubes with 164 passes per tube, and 30 ft long tubes. This amount of tube passes is impossible. To decrease the tube passes, a higher-pressure steam should be used. This would increase the LMTD and reduce the reboiler size. The purchase cost of the reboiler is $402,500.

Xylene Separation Distillation Column: S-501 (D-501, E-501, E-502A/B, P-501)

Unit ID: S-501	Temperature: 290ºF
Type: Distillation Column	Pressure: 30 psig
Material: Carbon Steel	Diameter: 16 ft
Specification Sheet: Section 16, pg. 110	Height: 64 ft
Costing Data: Section 17	Design Calculation: Section 25.3.4

The function of S-501 is to recover the desired xylene product and remove the undesirable hydrogen. A vapor stream, mostly containing xylene and isooctane, enters the column at 140,148 lb/hr, and three exit streams leave the column: liquid xylene, a liquid recycle stream, and a hydrogen-heavy vapor overhead. In the ASPEN simulation, this separation requires 16 stages, a feed at stage 5, a condenser pressure of 39 psig, a condenser pressure drop of 4 psig, a stage pressure drop of 0.12 psig, a reflux ratio of 5.7, and a bottoms flow rate of 79,418 lb/hr. ASPEN was used to obtain the height and diameter measurements of the column. With only one pass over the trays, the diameter is 16.3 feet, which can fit on a highway. This number of trays was used to calculate the height. It is industry standard to have 2 feet of spacing between each tray.

Additionally, a sump space of 4 feet was added, a headspace of 10 feet, a disengaging space of 3 feet, and a feed location spacing of 3 feet, were factored in. While ASPEN gives the theoretical number of stages, the actual number of trays was calculated through the O'Connell Correlation, which takes the efficiencies of the trays into account. This correlation indicates that there should be 23 trays, with a feed on tray 8, and a tray efficiency of 0.62. Therefore, the height of the column is 64 feet. This creates an L/D ratio of about 4. The total pressure drop over the column, calculated from ASPEN, is 1.2 psig. These calculations are also shown in the Appendix, Section 25.3.4. All parts of the column will be made out of carbon steel, again because the process fluid is non-corrosive and the temperature is within range of the material. The specification sheet is on page 110. The purchase cost of the column is $299,900.

The reflux accumulator, D-501, was designed as a horizontal pressure vessel. It was assumed that it would have a residence time of 5 min and an L/D ratio of 2. Using a flow of 483,527 lb/hr, the reflux accumulator will have a diameter of 11 ft and a height of 21 ft. The purchase cost of the reflux accumulator is $59,400.

The reflux pump, P-301, has a head of 84 ft, an isentropic efficiency of 0.747, and requires 16 hp. This was calculated by assuming a pressure drop of 20 psig and using equations in the Appendix, Section 25.3.1. The purchase cost of the reflux pump is $9,900, which will have a spare.

The partial condenser will be maintained at 100ºF by using 2,081,713 lb/hr of chilled water. According to ASPEN, the condenser has a heat duty of 101,916,000 BTU/hr. The heat transfer coefficient is 100 BTU/(ºF*ft^2*hr). Using the calculations in the Appendix, Section 25.3.2, the area of the condenser is 58,638 ft^2. Because of the large area, there should be two identical condensers in parallel. Assuming a tube velocity of 2 ft/sec, there will be 856 tubes with 8 passes per tube and 30 ft long tubes. The purchase cost of the condenser is $108,000.

The reboiler will be maintained at 367ºF by using very high-pressure steam of 1250 psig. According to ASPEN, the reboiler has a heat duty of 80,409,000 BTU/hr. The heat transfer coefficient is 150 BTU/(ºF*ft^2*hr). Using the calculations in the Appendix, Section 25.3.2, the area of the reboiler is 2,589 ft^2. Assuming a tube velocity of 2 ft/sec, there will be 46 tubes with 8 passes per tube, and 30 ft long tubes. The shell diameter will only be 15 inches.[26] The purchase cost of the reboiler is $101,100.

Hydrogen Separation Flash Drum: S-502

Unit ID: S-502	Temperature: 40ºF
Type: Flash Drum	Pressure: 285 psig
Material: Carbon Steel	Diameter: 18 ft
Specification Sheet: Section 16, pg. 111	Height: 53 ft
Costing Data: Section 17	Design Calculation: Section 25.3.5

The function of S-502 is to remove hydrogen from the process while minimizing loss of isobutylene, TMP, and isooctane. A mixed stream enters the flash at 17,902 lb/hr. Two streams exit: one as a liquid to get recycled, and one as a vapor mostly containing hydrogen to be burned. The drum runs at 40°F and 285 psig. The flash drum was sized using the equations in the Appendix, Section 25.3.5. With a hold-up time of 5 minutes to allow separation, the volume of gas in the drum was calculated to be 6,418 ft^3. It was assumed that the drum would be 50% full. Using these assumptions and an L/D ratio of 3, the diameter of the drum is 18 ft, and the height is 53 ft. The flash drum will be made of carbon steel because the fluid is non-corrosive and the temperature is within the range for carbon steel. The specification sheet is on page 111. The purchase cost of the reactor is $954,300.

Section 15.6 Storage Tanks

Isobutylene Storage Tank: T-101A/B

Unit ID: T-101	Temperature: 10ºF
Type: Storage Tank	Pressure: 5 psig
Material: Carbon Steel	Diameter/Tank: 23 ft
Specification Sheet: Section 16, pg. 112	Height/Tank: 70 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-101 is to store isobutylene. Isobutylene will be obtained via pipeline from the plant already on site. 126,820 lb/hr of isobutylene will enter the process. It will be refrigerated at 10ºF and stored at 5 psig. The fixed-roof tank will have a vent system to prevent pressure changes during filling and emptying. The storage tank should allow two days' worth of volume, so delivery is not too frequent. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of one month and the safety factor of 1.5, the volume of the tank will be 1.75 MM gal. Each storage tank should not exceed 1 MM gal, so there will be two storage tanks. Assuming an L/D ratio of 3, the diameter will be 23 ft and the height of the tank will be about 70 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. Because isobutylene is non-corrosive and at ambient temperature, the storage tank will be made of carbon steel. The specification sheet is on page 112. The purchase cost of the tank is $296,200. Additionally, the tank will use the already existing refrigeration, but utilities will need to maintain the low temperature. The use of a nitrogen blanket or a floating head tank should be explored due to flammability concerns.

Isooctane Storage Tank: T-102

Unit ID: T-102	Temperature: 80ºF
Type: Storage Tank	Pressure: 1 psig
Material: Carbon Steel	Diameter: 15 ft
Specification Sheet: Section 16, pg. 113	Height: 45 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-102 is to store isooctane. A vendor will deliver isooctane to the process area. For startup, 100,000 lb/hr of isooctane will need to enter the process. After that time, only the amount lost in the process through the three exit streams will need to be added to the process. This is about 445 lb/hr of isooctane. It can be stored at ambient conditions due to its very low boiling point of 210F. However, according to isooctane's MSDS sheet, it should be stored in a tightly sealed container due to flammability. The fixed-roof tank will have a vent system to prevent pressure changes during filling and emptying. The storage tank should allow three-weeks' worth of volume, so delivery is not too frequent. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of three weeks and the safety factor of 1.5, the volume of the tank will be 76,571 ft^3. Assuming an L/D ratio of 3, the diameter will be 15 ft and the height of the tank will be about 45 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. Because isooctane is non-corrosive and at ambient temperature, the storage tank will be made of carbon steel. The specification sheet is on page 113. The purchase cost of the tank is $124,900. The use of a nitrogen blanket should be explored due to flammability concerns.

Trimer Storage Tanks: T-301A/B

Unit ID: T-301A/B	Temperature: 80ºF
Type: Storage Tank	Pressure: 45 psig
Material: Carbon Steel	Diameter: 34 ft
Specification Sheet: Section 16, pg. 114	Height: 51 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-301 is to store trimers once they are taken out of the process. The storage tank should allow two days' worth of volume in case quality needs to be tested or the trimers cannot be transferred out of the plant immediately for some reason. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of two days and the safety factor of 1.5, the volume of the tank will be 91,956 ft^3 (697,023 gal). Assuming an L/D ratio of 3, the diameter will be 34 ft and the height of the tank will be about 102 ft. Because this is too tall, there will be two identical tanks, each with a diameter of 34 ft and a height of 51 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. The tank will be made of carbon steel because the trimers are non-corrosive. The specification sheet is on page 114. The purchase cost of the tank is $131,800. The use of a nitrogen blanket should be explored due to flammability concerns.

Xylene Storage Tanks: T-501A/B

Unit ID: T-501A/B	Temperature: 80ºF
Type: Storage Tank	Pressure: 20 psig
Material: Carbon Steel	Diameter: 36 ft
Specification Sheet: Section 16, pg. 115	Height: 53 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-501 is to store the xylene product once it has been created. The storage tank should allow two days' worth of volume in case quality needs to be tested or the xylene cannot be transferred out of the plant immediately for some reason. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of two days and the safety factor of 1.5, the volume of the tank will be 106,728 ft^3 (809,002 gal). Assuming an L/D ratio of 3, the diameter will be 36 ft and the height of the tank will be about 107 ft. Because this is too tall, there will be two identical tanks, each with a diameter of 36 ft and a height of 53 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. The tank will be made of carbon steel because xylene is non-corrosive. The specification sheet is on page 115. The purchase cost of the tank is $142,150. The use of a nitrogen blanket should be explored due to flammability concerns.

Section 15.7 Surge Tanks

Surge Tanks After S-301: T-302A/B

Unit ID: T-302A/B	Temperature: 240ºF
Type: Surge Tank	Pressure: 55 psig
Material: Carbon Steel	Diameter: 38 ft
Specification Sheet: Section 16, pg. 116	Height: 57 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-302 is to provide intermediate storage after the first half of the process has been completed; therefore, the second half of the process can continue if the first half is down. The surge tank should allow one-day worth of volume. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of one day and the safety factor of 1.5, the volume of the tank will be 130,680 ft^3 (990,554 gal). Assuming an L/D ratio of 3, the diameter will be 38 ft and the height of the tank will be about 114 ft. Because this is too tall, there will be two identical tanks, each with a diameter of 38 ft and a height of 57 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. The tank will be made of carbon steel because the fluids are non-corrosive. The specification sheet is on page 116. The purchase cost of the tank is $449,000. The use of a nitrogen blanket should be explored due to flammability concerns.

Recycle Surge Tanks: T-502A/B

Unit ID: T-302A/B	Temperature: 87ºF
Type: Surge Tank	Pressure: 24 psig
Material: Carbon Steel	Diameter: 27 ft
Specification Sheet: Section 16, pg. 118	Height: 40 ft
Costing Data: Section 17	Design Calculation: Section 25.3.6

The function of T-502 is to provide intermediate storage of the recycle stream. The surge tank should allow one-day worth of volume. It was assumed that the tank should allow a capacity of 1.5 times the amount needed. Using the time capacity of one day and the safety factor of 1.5, the volume of the tank will be 46,620 ft^3 (353,380 gal). Assuming an L/D ratio of 3, the diameter will be 27 ft and the height of the tank will be about 81 ft. Because this is too tall, there will be two identical tanks, each with a diameter of 27 ft and a height of 40 ft. Due to the large volume of the tank, it will be built on site, which is industry standard for storage tanks. Sections of the tank's wall will be delivered to the site by barge. The tank will be made of carbon steel because the fluids are non-corrosive. The specification sheet is on page 118. The purchase costs of the tanks are $283,050. The use of a nitrogen blanket should be explored due to flammability concerns.

Section 16
Specification Sheets

Isobutylene Pump

Identification:	**Item**	*Isooctane Pump*	Date: *17 April 2018*
	Item No.	P-101	By: *MTN*
	No. required	1	

Function: Pressurize fresh isobutylene.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	10	10
Pressure (psig)	5	24
Vapor fraction	0	0
Mass flow (lb/hr)	126820	126820
Molar flow (lbmol/hr)	2260	2260
Component Mass Flow (lb/hr)		
Isobutylene	126820	126820
para-Xylene	0	0
Isooctane	0	0
2,4,4-trimethylpentene	0	0
Trimers	0	0
meta-Xylene	0	0
ortho-Xylene	0	0
Hydrogen	0	0

Design Data:

Net Work: 10.8 hp
Material of Construction: Carbon Steel
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: VSC
Flowrate: 400 gpm
Head: 73 ft
Max Motor hp: 75

Annual Utilities: Electricity at 4,703 kWh.

Comments and drawings: See Section 12 Process Flow Sheet Section 100

Isooctane Pump

Identification:	**Item**	*Isooctane Pump*	Date: *17 April 2018*
	Item No.	P-102	By: *MTN*
	No. required	1	

Function: Pressurize fresh isooctane.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	80	80
Pressure (psig)	0.3	24
Vapor fraction	0	0
Mass flow (lb/hr)	445.37	445.37
Molar flow (lbmol/hr)	4	4
Component Mass Flow (lb/hr)		
Isobutylene	0	0
para-Xylene	0	0
Isooctane	445.37	445.37
2,4,4-trimethylpentene	0	0
Trimers	0	0
meta-Xylene	0	0
ortho-Xylene	0	0
Hydrogen	0	0

Design Data:

Net Work: 0.05 hp
Material of Construction: Carbon Steel
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: VSC
Flowrate: 1.3 gpm
Head: 69 ft
Max Motor hp: 75

Annual Utilities: Electricity at 192 kWh.

Comments and drawings: See Section 12 Process Flow Sheet Section 100

R-201 Feed Pump

Identification:	**Item**	*R-201 Feed Pump*	Date: *17 April 2018*
	Item No.	P-103	By: *MTN*
	No. required	1	

Function: Pressurize feed to R-201.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	31	39
Pressure (psig)	5.3	750
Vapor fraction	0	0
Mass flow (lb/hr)	181998	181998
Molar flow (lbmol/hr)	2755	2755
Component Mass Flow (lb/hr)		
Isobutylene	127890	127890
p-Xylene	743	743
Isooctane	43394	43394
2,4,4-trimethylpentene	9920.5	9920.5
Trimers	0	0
meta-Xylene	36	36
ortho-Xylene	14	14
Hydrogen	0.5	0.5

Design Data:

Net Work: 337 hp
Material of Construction: Carbon Steel
No. Stages: 2+
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: HSC
Flowrate: 586 gpm
Head: 2,750 ft
Max Motor hp: 1,450

Annual Utilities: Electricity at 1,613,450 kWh

Comments and drawings: See Section 12 Process Flow Sheet Section 100

R-201 Recirculation Pump

Identification:	**Item**	*R-201 Recirc Pump*	Date: *17 April 2018*
	Item No.	P-201	By: *MTN*
	No. required	1	

Function: Re-pressurize mixture in R-201 recirculation loop.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	372	372
Pressure (psig)	750	770
Vapor fraction	0	0
Mass flow (lb/hr)	895140	895104
Molar flow (lbmol/hr)	7438	7438
Component Mass Flow (lb/hr)		
Isobutylene	11591	11591
para-Xylene	3654	3654
Isooctane	213348	213348
2,4,4-trimethylpentene	460455	460455
Trimers	205842	205842
meta-Xylene	178	178
ortho-Xylene	69	69
Hydrogen	2	2

Design Data:

Net Work: 47 hp
Material of Construction: Carbon Steel
No. Stages: 1
Shaft rpm: 1800
Type: Centrifugal Pump
Orientation: HSC
Flowrate: 3,244 gpm
Head: 84 ft
Max Motor hp: 250

Annual Utilities: Electricity at 213,419 kWh

Comments and drawings: See Section 12 Process Flow Sheet Section 200

R-401 Recirculation Blower

Identification:	**Item**	*R-401 Recirculation Blower*	Date: *17 April 2018*
	Item No.	C-401	By: *MTN*
	No. required	1	

Function: Re-pressurize mixture in R-401 recirculation loop.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	1001	1022
Pressure (psig)	22	30
Vapor fraction	1	1
Mass flow (lb/hr)	1610150	1610150
Molar flow (lbmol/hr)	40001	40001
Component Mass Flow (lb/hr)		
Isobutylene	27089	27089
para-Xylene	820401	820401
Isooctane	496117	496117
2,4,4-trimethylpentene	114702	114702
Trimers	9625	9625
meta-Xylene	45519	45519
ortho-Xylene	45265	45265
Hydrogen	51431	46955

Design Data:

Net Work: 11,009 hp
Material of Construction: Stainless Steel
Isentropic Efficiency: 0.85
Constant Specific Heat Ratio: 1.4

Annual Utilities: Electricity at 64,670,076 kWh

Comments and drawings: Designed by AirPro Fan & Blower Company. See Section 12 Process Flow Sheet Section 400

S-502 Compressor

Identification:	**Item**	*S-502 Compressor*	Date: *17 April 2018*
	Item No.	C-501	By: *MTN*
	No. required	1	

Function: Pressurize feed into Flash drum.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	100	454
Pressure (psig)	24	285
Vapor fraction	1	1
Mass flow (lb/hr)	17902.6	17902.6
Molar flow (lbmol/hr)	2358	2358
Component Mass Flow (lb/hr)		
Isobutylene	2146	2146
para-Xylene	38	38
Isooctane	9251	9251
2,4,4-trimethylpentene	1987	1987
Trimers	0	0
meta-Xylene	2	2
ortho-Xylene	0.6	0.6
Hydrogen	4476	4476

Design Data:

Net Work: 3207 hp
Material of Construction: Carbon Steel
No. Stages: 3
No. Intercoolers: 2
Net Heat Duty:
Type: Multistage Compressor
Isentropic Efficiency: 0.85 per stage
Overall Compression ratio: 12 (1st stage: 3; 2nd stage: 3, 3rd stage: 2)

Annual Utilities: Electricity at 13,266,146 kWh

Comments and drawings: See Section 12 Process Flow Sheet Section 500

C-501 Intercooler

Identification:	**Item**	*C-501 Intercooler*	Date: *17 April 2018*
	Item No.	C-501A	By: *MTN*
	No. required	1	

Function: Cool down mixture between compressor stages.

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	80	100	224	150
Pressure (psig)	10	0	70	70
Vapor fraction	0	0	1	1
Mass flow (lb/hr)	80085	80085	17902.6	17902.6
Molar flow (lbmol/hr)	445	445	2358	2358
Component Mass Flow (lb/hr)				
Isobutylene	0	0	2146	2146
para-Xylene	0	0	38	38
Isooctane	0	0	9251	9251
2,4,4-trimethylpentene	0	0	1987	1987
Trimers	0	0	0	0
meta-Xylene	0	0	2	2
ortho-Xylene	0	0	0.6	0.6
Hydrogen	0	0	4476	4476
Cooling Water	80085	80085	0	0

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area/unit: 170 ft^2
LMTD: 94ºF
Heat Exchanged: 1,601,657 BTU/hr
Heat Transfer Coeff: 100 BTU/(hr*ft^2*ºF)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass:
Tube Length:
No. of Tube Passes:
Baffle Spacing:
Shell Diameter:

Utilities: 80,085 lb/hr of cooling water

Comments and drawings: Cooling water on the tube side, Hot process fluid on the shell side. See Section 12 Process Flow Sheet Section 500

C-501 Intercooler

Identification:	**Item**	*C-501 Intercooler*	Date: *17 April 2018*
	Item No.	C-501B	By: *MTN*
	No. required	1	

Function: Cool down mixture between compressor stages.

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	80	100	340	200
Pressure (psig)	0	24	200	200
Vapor fraction	0	0	1	1
Mass flow (lb/hr)	140000	140000	17902.6	17902.6
Molar flow (lbmol/hr)	7771	7771	2358	2358
Component Mass Flow (lb/hr)				
Isobutylene	0	0	2146	2146
para-Xylene	0	0	38	38
Isooctane	0	0	9251	9251
2,4,4-trimethylpentene	0	0	1987	1987
Trimers	0	0	0	0
meta-Xylene	0	0	2	2
ortho-Xylene	0	0	0.6	0.6
Hydrogen	0	0	4476	4476
Cooling Water	140000	140000	0	0

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area:
Heat Exchanged: BTU/hr
Heat Transfer Coeff: BTU/(hr*ft^2*°F)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass:
Tube Length:
No. of Tube Passes:
Baffle Spacing:
Shell Diameter:

Utilities: 140,000 lb/hr of cooling water

Comments and drawings: Cooling water on the tube side, Hot process fluid on the shell side. See Section 12 Process Flow Sheet Section 500

R-201 Feed Heat Exchanger

Identification:	**Item**	*R-201 Feed HX*	Date: *17 April 2018*
	Item No.	E-101	By: *MTN*
	No. required	1	

Function: Heat R-201 feed

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	39	347	366	366
Pressure (psig)	750	750	150	150
Vapor fraction	0	0	1	0
Mass flow (lb/hr)	181998	181998	70332	70332
Molar flow (lbmol/hr)	2755	2755		
Component Mass Flow (lb/hr)				
Isobutylene	127890	127890	0	0
para-Xylene	743	743	0	0
Isooctane	43394	43394	0	0
2,4,4-trimethylpentene	9920.5	9920.5	0	0
Trimers	0	0	0	0
meta-Xylene	36	36	0	0
ortho-Xylene	14	14	0	0
Hydrogen	0.5	0.5	0	0
lps (150 psig)	0	0	70332	70332

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area: 2,977 ft^2
LMTD: 108ºF
Heat Exchanged: 48,224,400BTU/hr
Heat Transfer Coeff: 150 BTU/(hr*ft^2*ºF)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass: 78
Tube Length: 24 ft
No. of Tube Passes: 6
Shell Diameter: 37 in

Utilities: 70,332 lb/hr of low pressure steam at 150 psig

Comments and drawings: Process fluid on the tube side, Low pressure steam on the shell side. See Section 12 Process Flow Sheet Section 100

R-201 Recirculation Heat Exchanger

Identification:	**Item**	*R-201 Recirc HX*	Date: *17 April 2018*
	Item No.	E-201	By: *MTN*
	No. required	1	

Function: Cool R-201 recirculation loop.

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	80	105	372	300
Pressure (psig)	10	0	770	770
Vapor fraction	0	0	0	0
Mass flow (lb/hr)	1836975	1836975	895104	895140
Molar flow (lbmol/hr)	101968	101968	7438	7438
Component Mass Flow (lb/hr)				
Isobutylene	0	0	11591	11591
para-Xylene	0	0	3654	3654
Isooctane	0	0	213348	213348
2,4,4-trimethylpentene	0	0	460455	460455
Trimers	0	0	205842	205842
meta-Xylene	0	0	178	178
ortho-Xylene	0	0	69	69
Hydrogen	0	0	2	2
Cooling Water	1836975	1836975	0	0

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area:1,892 ft^2
LMTD: 243°F
Heat Exchanged: 45,923,300 BTU/hr
Heat Transfer Coeff: 100 BTU/(hr*ft^2*°F)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass: 189
Tube Length: 24 ft
No. of Tube Passes: 2
Baffle Spacing: 22.2 inches
Shell Diameter: 37 inches

Utilities: 1,836,975 lb/hr of cooling water

Comments and drawings: Cooling water on the tube side, Hot process fluid on the shell side. See Section 12 Process Flow Sheet Section 200

Trimer Stream Heat Exchanger

Identification:	**Item**	*Trimer Stream HX*	Date: *17 April 2018*
	Item No.	E-303	By: *MTN*
	No. required	1	

Function: Cool trimer product stream

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	80	105	543	90
Pressure (psig)	10	0	58	45
Vapor fraction	0	0	0	0
Mass flow (lb/hr)	483548	483548	41852	41852
Molar flow (lbmol/hr)	26841	26841	251	251
Component Mass Flow (lb/hr)				
Isobutylene	0	0	0	0
para-Xylene	0	0	56	56
Isooctane	0	0	209	209
2,4,4-trimethylpentene	0	0	568	568
Trimers	0	0	41015	41015
meta-Xylene	0	0	3	3
ortho-Xylene	0	0	2	2
Hydrogen	0	0	0	0
Cooling Water	483548	483548	0	0

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area: 1,085 ft^2
LMTD: 113°F
Heat Exchanged: 12,291,800 BTU/hr
Heat Transfer Coeff: 100 BTU/(hr*ft^2*°F)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass: 80
Tube Length: 24 ft
No. of Tube Passes: 2
Baffle Spacing: 18.6 inches
Shell Diameter: 21¼ inches

Utilities: 483,548 lb/hr of cooling water

Comments and drawings: Cooling water on the tube side, Hot process fluid on the shell side. See Section 12 Process Flow Sheet Section 300

R-401 Feed Heat Exchanger

Identification:	**Item**	*R-401 Feed HX*	Date: *17 April 2018*
	Item No.	E-401	By: *MTN*
	No. required	1	

Function: Heat up R-401 feed while simultaneously cooling R-401 effluent.

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	240	856	1022	240
Pressure (psig)	55	55	30	20
Vapor fraction	0	1	1	1
Mass flow (lb/hr)	140148	10148	140148	140148
Molar flow (lbmol/hr)	1261	1261	3482	3482
Component Mass Flow (lb/hr)				
Isobutylene	2356	2356	2358	2358
para-Xylene	687	687	71408	71408
Isooctane	43168.5	43168.5	43182	43182
2,4,4-trimethylpentene	93052	93052	9984	9984
Trimers	837	837	838	838
meta-Xylene	33	33	3962	3962
ortho-Xylene	12	12	3940	3940
Hydrogen	0.5	0.5	4477	4477

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area: 16,350 ft^2
LMTD: 96ºF
Heat Exchanged: 35,434,800 BTU/hr
Heat Transfer Coeff: 45 BTU/(hr*ft^2*ºF)
Tube Side Material of Construction: Stainless Steel 304
Shell Side Material of Construction: Stainless Steel 304
No. Tubes/Pass: 92
Tube Length: 30 ft
No. of Tube Passes: 23*

Comments and drawings: See Section 12 Process Flow Sheet Section 400

Xylene Stream Heat Exchanger

Identification:	**Item**	*Xylene Stream HX*	Date: *17 April 2018*
	Item No.	E-503	By: *MTN*
	No. required	1	

Function: Cool xylene product stream

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	80	105	367	90
Pressure (psig)	10	0	30	20
Vapor fraction	0	0	0	0
Mass flow (lb/hr)	451564	451564	79418	79418
Molar flow (lbmol/hr)	25066	25066	745	745
Component Mass Flow (lb/hr)				
Isobutylene	0	0	0	0
para-Xylene	0	0	70665	70665
Isooctane	0	0	38	38
2,4,4-trimethylpentene	0	0	25	25
Trimers	0	0	838	838
meta-Xylene	0	0	3926	3926
ortho-Xylene	0	0	3926	3926
Hydrogen	0	0	0	0
Cooling Water	451564	451564	0	0

Design Data:

Type: Shell-in-Tube, Fixed Head
Effective Surface Area: 1,467 ft^2
LMTD: 77ºF
Heat Exchanged: 11,291,500 BTU/hr
Heat Transfer Coeff: 100 BTU/(hr*ft^2*ºF)
Tube Side Material of Construction: Carbon Steel
Shell Side Material of Construction: Carbon Steel
No. Tubes/Pass: 75
Tube Length: 24 ft
No. of Tube Passes: 4
Baffle Spacing: 18.6 inches
Shell Diameter: 31 inches

Utilities: 451,564 lb/hr of cooling water

Comments and drawings: Cooling water on the tube side, Hot process fluid on the shell side. See Section 12 Process Flow Sheet Section 500

R-401 Recirculation Furnace

Identification:	**Item**	*R-401 Recirc Furnace*	Date: *17 April 2018*
	Item No.	E-402	By: *MTN*
	No. required	1	

Function: Heat R-401 recirculation loop

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out
Temperature (°F)	1022	1050	Flue Gas	Flue Gas
Pressure (psig)	30	30	--	--
Vapor fraction	1	1	1	1
Mass flow (lb/hr)	1470000	1470000	1407	1407
Molar flow (lbmol/hr)	36519	36519	88	88
Component Mass Flow (lb/hr)				
Isobutylene	24731	24731	0	0
para-Xylene	748993	748993	0	0
Isooctane	452934	452934	0	0
2,4,4-trimethylpentene	104719	104719	0	0
Trimers	8787	8787	0	0
meta-Xylene	41557	41557	0	0
ortho-Xylene	41325	41325	0	0
Hydrogen	46954	46954	0	0
Methane	0	0	1407	1407

Design Data:

Type: Fired heater
Heat Exchanged: 33,355,300 BTU/hr
Pressure: 30 psig

Utilities: 1,407 lb/hr of methane

Comments and drawings: See Section 12 Process Flow Sheet Section 400

Oligomerization Reactor

Identification:	**Item**	*Oligomerization Reactor*	Date: *17 April 2018*
	Item No.	R-201	By: *MTN*
	No. required	1	

Function: Allow reactions to take place to form desired intermediate, TMP, and undesired byproduct, trimers.

Operation: Continuous

Materials handled:	Feed	Effluent
Temperature (°F)	307	372
Pressure (psig)	750	750
Vapor fraction	0	0
Mass flow (lb/hr)	1077140	1077140
Molar flow (lbmol/hr)	10194	8951
Component Mass Flow (lb/hr)		
Isobutylene	139482	13948
para-Xylene	4398	4398
Isooctane	256726	256726
2,4,4-trimethylpentene	470386	554075
Trimers	205849	247694
meta-Xylene	214	214
ortho-Xylene	82	82
Hydrogen	3	3

Design Data:

Adiabatic Temperature Rise: 65ºF
Mass catalyst: 71,809 lb
Material of Construction: Carbon Steel
Inner diameter: 8 ft
Total Height: 33 ft
Total Reactor Volume: 1,745 ft^3
Orientation: Vertical
Total Residence Time: 3.44 min
Superficial Fluid Velocity: 0.16 ft/s

Utilities: Exothermic reactions release 15,429,951 BTU/hr

Comments and drawings: See Section 12 Process Flow Sheet Section 200

Dehydrocyclization Reactors

Identification:	**Item**	*Dehydrocyclization Reactor*	Date: *17 April 2018*
	Item No.	R-401	By: *MTN*
	No. required	4	

Function: Allow reactions to take place to form desired product, p-xylene, and undesired isomers, o-xylene and m-xylene.

Operation: Continuous

Materials handled:	Overall Feed	Overall Effluent
Temperature (°F)	1034	1001
Pressure (psig)	30	22
Vapor fraction	1	1
Mass flow (lb/hr)	1610150	1610150
Molar flow (lbmol/hr)	37780	40001
Component Mass Flow (lb/hr)		
Isobutylene	27089	27089
para-Xylene	749675	820401
Isooctane	496117	496117
2,4,4-trimethylpentene	197763	114702
Trimers	9625	9625
meta-Xylene	41590	45519
ortho-Xylene	41336	45265
Hydrogen	46955	51431

Design Data:

Adiabatic Temperature Drop: 33ºF
Mass catalyst/unit: 487,924 lb
Material of Construction: SS 304
Height/unit: 65 ft
Diameter/unit: 16 ft
Total Reactor Volume: 40,234 ft^3
Reactor Volume/unit: 13,411 ft^3
No. units in parallel: 3
Orientation: Vertical
Superficial Fluid Velocity: 6.92 ft/s
Total Residence Time: 0.256 min

Utilities: Endothermic reactions require 40,874,883 BTU/hr

Comments and drawings: See Section 12 Process Flow Sheet Section 400; Assume reaction conversion is evenly spread out over all units; 3 reactors will be operating at once with a 4th swing reactor undergoing catalyst regeneration, allowing less downtime; The adiabatic temperature drop is reasonable.

Trimer Separation Distillation Column

Identification:	**Item**	*Trimer Sep Dist Column*	Date: *17 April 2018*
	Item No.	S-301	By: *MTN*
	No. required	1	

Function: Separate out trimers from process stream.

Operation: Continuous

Materials handled:	Feed	Liquid Dist.	Bottoms
Temperature (°F)	355	240	543
Pressure (psig)	65	55	58
Vapor fraction	0	0	0
Mass flow (lb/hr)	182000	140148	41852
Molar flow (lbmol/hr)	1512	1261	251
Component Mass Flow (lb/hr)			
Isobutylene	2357	2356	0
para-Xylene	743	687	56
Isooctane	43378.5	43168.5	209
2,4,4-trimethylpentene	93620	93052	568
Trimers	41852	837	41015
meta-Xylene	36	33	3
ortho-Xylene	14	12	2
Hydrogen	0.5	0.5	0

Design Data:

Number of trays: 17
Feed Stage: 11
Pressure: 65 psig
Temperature: 355 ºF
Total Height: 44 ft
Material of Construction: Carbon Steel
Diameter: 9 ft
Average Tray Efficiency: 0.44
Tray Spacing: 1.5 ft
Skirt Height: 17 ft
Reflux Ratio: 0.165

Utilities: Cooling water at 1,081,117 lb/hr and 1250 psig steam at 33,219 lb/hr.

Comments and drawings: See Section 12 Process Flow Sheet Section 400

Xylene Separation Distillation Column

Identification:	**Item**	*Xylene Sep Dist Column*	Date: *17 April 2018*
	Item No.	S-501	By: *MTN*
	No. required	1	

Function: Separate out xylene and hydrogen from the process stream.

Operation: Continuous

Materials handled:	Feed	Liquid Dist.	Vapor Dist.	Bottoms
Temperature (°F)	240	100	100	367
Pressure (psig)	30	24	24	30
Vapor fraction	1	0	1	0
Mass flow (lb/hr)	140148	42892.1	17902.6	79418
Molar flow (lbmol/hr)	3482	379	2358	745
Component Mass Flow (lb/hr)				
Isobutylene	2358	211	2146	0
para-Xylene	71408	705	38	70665
Isooctane	43182	33894	9251	38
2,4,4-trimethylpentene	9984	7971	1987	25
Trimers	838	0	0	838
meta-Xylene	3962	34	2	3926
ortho-Xylene	3940	13	0.6	3926
Hydrogen	4477	0.1	4476	0

Design Data:

Number of trays: 23
Feed Stage: 6
Pressure: 30 psig
Temperature: 290 ºF
Total Height: 64 ft
Material of Construction: Carbon Steel
Diameter: 16 ft
Average Tray Efficiency: 0.62
Tray Spacing: 1.5 ft
Skirt Height: 17 ft
Reflux Ratio: 1.42

Utilities: Cooling water at 2,081,713 lb/hr and 1250 psig steam at 139,357 lb/hr.

Comments and drawings: See Section 12 Process Flow Sheet Section 500

Hydrogen Separation Flash Drum

Identification:	**Item**	*Hydrogen Sep Flash Drum*	Date: *17 April 2018*
	Item No.	S-502	By: *MTN*
	No. required	1	

Function: Remove undesired hydrogen from process stream.

Operation: Continuous

Materials handled:	Feed	Vapor Exit	Liquid Exit
Temperature (°F)	50	40	40
Pressure (psig)	285	285	285
Vapor fraction	0.95	1	0
Mass flow (lb/hr)	17902	5997	11905
Molar flow (lbmol/hr)	2358	2245	112
Component Mass Flow (lb/hr)			
Isobutylene	2146	1288	859
para-Xylene	38	0	38
Isooctane	9251	196	9055
2,4,4-trimethylpentene	1987	38	1950
Trimers	0	0	0
meta-Xylene	2	0	2
ortho-Xylene	1	0	1
Hydrogen	4476	4476	0

Design Data:

Hold-up time: 5 min
Pressure: 285 psig
Total Height: 53 ft
Material of Construction: Carbon Steel
Diameter: 18 ft
Orientation: Vertical
Fraction of Drum Full: 50%

Comments and drawings: See Section 12 Process Flow Sheet Section 500

Isobutylene Storage Tanks

Identification:	**Item**	*Isobutylene Storage Tank*	Date: *17 April 2018*
	Item No.	T-101A/B	By: *MTN*
	No. required	2	

Function: Store excess isobutylene.

Operation: Continuous

Materials handled:	To Process
Temperature (°F)	10
Pressure (psig)	5
Vapor fraction	0
Mass flow (lb/hr)	126820
Molar flow (lbmol/hr)	2260
Component Mass Flow (lb/hr)	
Isobutylene	126820
para-Xylene	0
Isooctane	0
2,4,4-trimethylpentene	0
Trimers	0
meta-Xylene	0
ortho-Xylene	0
Hydrogen	0

Design Data:

Amount (time) of Isobutylene Stored: 2 days

Diameter: 23 ft

Height/Unit: 70 ft

Material of Construction: Carbon Steel

Roof Design: Conical

Pressure: 5 psig

Total Storage Volume/Tank: 115,511 ft^3; 875,571 gal

Comments and drawings: See Section 12 Process Flow Sheet Section 100

Isooctane Storage Tank

Identification:	**Item**	*Isooctane Storage Tank*	Date: *17 April 2018*
	Item No.	T-102	By: *MTN*
	No. required	1	

Function: Store excess isooctane.

Operation: Continuous

Materials handled:	To Process
Temperature (°F)	80
Pressure (psig)	0.3
Vapor fraction	0
Mass flow (lb/hr)	445.37
Molar flow (lbmol/hr)	4
Component Mass Flow (lb/hr)	
Isobutylene	0
para-Xylene	0
Isooctane	445.37
2,4,4-trimethylpentene	0
Trimers	0
meta-Xylene	0
ortho-Xylene	0
Hydrogen	0

Design Data:

Amount (time) of Isooctane Stored: 3 weeks

Diameter: 15 ft
Height: 45 ft

Material of Construction: Carbon Steel
Roof Design: Conical

Pressure: 0.3 psig

Total Storage Volume: 7,820 ft^3; 59,277 gallons

Comments and drawings: See Section 12 Process Flow Sheet Section 100

Trimer Storage Tanks

Identification:	**Item**	*Trimer Storage Tank*	Date: *17 April 2018*
	Item No.	T-301A/B	By: *MTN*
	No. required	2	

Function: Store trimer product.

Operation: Continuous

Materials handled:	To Tank
Temperature (°F)	90
Pressure (psig)	45
Vapor fraction	0
Mass flow (lb/hr)	41852
Molar flow (lbmol/hr)	251
Component Mass Flow (lb/hr)	
Isobutylene	0
para-Xylene	56
Isooctane	209
2,4,4-trimethylpentene	568
Trimers	41015
meta-Xylene	3
ortho-Xylene	2
Hydrogen	0

Design Data:

Amount (time) of Trimers Stored: 2 days
Diameter: 34 ft
Height/Unit: 51 ft
Material of Construction: Carbon Steel
Roof Design: Conical
Pressure: 45 psig
Total Storage Volume: 91,956 ft^3; 697,023 gallons

Comments and drawings: See Section 12 Process Flow Sheet Section 300

Xylene Storage Tanks

Identification:	**Item**	*Xylene Storage Tank*	Date: *17 April 2018*
	Item No.	T-501A/B	By: *MTN*
	No. required	2	

Function: Store xylene product.

Operation: Continuous

Materials handled:	To Tank
Temperature (°F)	90
Pressure (psig)	20
Vapor fraction	0
Mass flow (lb/hr)	79418
Molar flow (lbmol/hr)	745
Component Mass Flow (lb/hr)	
Isobutylene	0
para-Xylene	70665
Isooctane	38
2,4,4-trimethylpentene	25
Trimers	838
meta-Xylene	3926
ortho-Xylene	3926
Hydrogen	0

Design Data:

Amount (time) of Xylene Stored: 2 days

Diameter: 36 ft
Total height: 53 ft

Material of Construction: Carbon Steel
Roof Design: Conical

Pressure: 20 psig

Total Storage Volume: 106,728 ft^3; 809,002 gal

Comments and drawings: See Section 12 Process Flow Sheet Section 500

Surge Tanks After S-301

Identification:	**Item**	*Surge Tank After S-301*	Date: *17 April 2018*
	Item No.	T-302A/B	By: *MTN*
	No. required	2	

Function: Process stream fills tank to split process into multiple parts, so part of process can continue if another part is shutdown.

Operation: Continuous

Materials handled:	To Tank	Inside Tank
Temperature (°F)	240	240
Pressure (psig)	55	15
Vapor fraction	0	0
Mass flow (lb/hr)	140148	140148
Molar flow (lbmol/hr)	1261	1261
Component Mass Flow (lb/hr)		
Isobutylene	2356	2356
para-Xylene	687	687
Isooctane	43168.5	43168.5
2,4,4-trimethylpentene	93052	93052
Trimers	837	837
meta-Xylene	33	33
ortho-Xylene	12	12
Hydrogen	0.5	0.5

Design Data:

Amount (time) of Process Stream Stored: 1 day
Diameter: 38 ft
Total height: 57 ft
Material of Construction: Carbon Steel
Roof Design: Conical
Pressure: 15 psig
Total Storage Volume: 130,680 ft^3; 990,554 gal

Comments and drawings: See Section 12 Process Flow Sheet Section 300

T-302 Pump

Identification:	**Item**	*T-302 Pump*	Date: *17 April 2018*
	Item No.	P-302	By: *MTN*
	No. required	1	

Function: Pressurize process stream after surge tank.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	240	240
Pressure (psig)	15	55
Vapor fraction	0	0
Mass flow (lb/hr)	140148	140148
Molar flow (lbmol/hr)	1261	1261
Component Mass Flow (lb/hr)		
Isobutylene	2356	2356
para-Xylene	687	687
Isooctane	43168.5	43168.5
2,4,4-trimethylpentene	93052	93052
Trimers	837	837
meta-Xylene	33	33
ortho-Xylene	12	12
Hydrogen	0.5	0.5

Design Data:

Net Work: 11 hp
Material of Construction: Carbon Steel
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: VSC
Flowrate: 453 gpm
Head: 97 ft

Utilities: Electricity at 46,952 kWh

Comments and drawings: See Section 12 Process Flow Sheet Section 300

Recycle Stream Surge Tanks

Identification:	**Item**	*Recycle Stream Surge Tank*	Date: *17 April 2018*
	Item No.	T-502A/B	By: *MTN*
	No. required	2	

Function: Recycle stream fills tank to split process into multiple parts, so part of process can continue if another part is shutdown.

Operation: Continuous

Materials handled:	To Tank	Inside Tank
Temperature (°F)	87	87
Pressure (psig)	24	0
Vapor fraction	0	0
Mass flow (lb/hr)	54733	54733
Molar flow (lbmol/hr)	491	491
Component Mass Flow (lb/hr)		
Isobutylene	1070	1070
para-Xylene	743	743
Isooctane	42949	42949
2,4,4-trimethylpentene	9920.5	9920.5
Trimers	0	0
meta-Xylene	36	36
ortho-Xylene	14	14
Hydrogen	0.5	0.5

Design Data:

Amount (time) of Recycle Stream Stored: 1 day
Diameter: 27 ft
Total height: 40 ft
Material of Construction: Carbon Steel
Roof Design: Conical
Pressure: 0 psig
Total Storage Volume: 46,620 ft^3; 353,380 gal

Comments and drawings: See Section 12 Process Flow Sheet Section 500

T-502 Pump

Identification:	**Item**	*T-502 Pump*	Date: *17 April 2018*
	Item No.	P-501	By: *MTN*
	No. required	1	

Function: Pressurize recycle stream after surge tank.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	87	87
Pressure (psig)	0	15
Vapor fraction	0	0
Mass flow (lb/hr)	54733	54733
Molar flow (lbmol/hr)	491	491
Component Mass Flow (lb/hr)		
Isobutylene	1070	1070
para-Xylene	743	743
Isooctane	42949	42949
2,4,4-trimethylpentene	9920.5	9920.5
Trimers	0	0
meta-Xylene	36	36
ortho-Xylene	14	14
Hydrogen	0.5	0.5

Design Data:

Net Work: 4 hp
Material of Construction: Carbon Steel
No. Stages: 1
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: VSC
Flowrate: 159 gpm
Head: 82 ft

Utilities: Electricity at 19,208 kWh

Comments and drawings: See Section 12 Process Flow Sheet Section 500

Section 17
Equipment Cost Summary

Table 17.1 Equipment Cost of Storage Equipment and Process Machinery

Unit ID	Type	Purchase Cost ($)	Bare Module Factor	Bare Module Cost ($)	Unit Type	Description
T-101A	Storage	$296,200	3.21	$950,900	Storage Tank	Isobutylene Storage Tank A
T-101B	Storage	$296,200	3.21	$950,900	Storage Tank	Isobutylene Storage Tank B
T-102	Storage	$124,900	3.21	$400,900	Storage Tank	Isooctane Storage Tank
T-301	Storage	$263,600	3.21	$846,100	Storage Tank	Trimer Storage Tank
T-501	Storage	$284,300	3.21	$912,500	Storage Tank	Xylene Storage Tank
T-302	Storage	$315,600	4.16	$1,322,000	Surge Tank	Surge Tank After S-301
T-502	Storage	$186,000	4.16	$773,700	Surge Tank	Recycle Stream Surge Tank
P-101	Process Machinery	$32,000	3.30	$105,700	Pump	Isooctane Pump
P-10X	Spare	$32,000	3.30	$105,700	Spare Pump	Spare Isooctane Pump
P-102	Process Machinery	$189,900	3.30	$626,500	Pump	R-201 Feed Pump
P-10X	Spare	$189,900	3.30	$626,500	Spare Pump	Spare R-201 Feed Pump
P-103	Process Machinery	$8,000	3.30	$26,400	Pump	Isobutylene Pump
P-10X	Spare	$8,000	3.30	$26,400	Spare Pump	Spare Isobutylene Pump
P-201	Process Machinery	$41,700	3.30	$137,700	Pump	R-201 Recirculation Pump
P-20X	Spare	$41,700	3.30	$137,700	Spare Pump	Spare R-201 Recirculation Pump
P-301	Process Machinery	$9,000	3.30	$29,600	Pump	Trimer Column Reflux Pump
P-30X	Spare	$9,000	3.30	$29,600	Spare Pump	Spare Trimer Column Reflux Pump
P-302	Process Machinery	$6,800	3.30	$22,500	Pump	T-302 Pump
P-30X	Spare	$6,800	3.30	$22,500	Spare Pump	Spare T-302 Pump
P-501	Process Machinery	$10,000	3.30	$32,700	Pump	Xylene Column Reflux Pump
P-50X	Spare	$10,000	3.30	$32,700	Spare Pump	Spare Xylene Column Reflux Pump
P-502	Process Machinery	$8,600	3.30	$28,400	Pump	T-502 Pump
P-50X	Spare	$8,600	3.30	$28,400	Spare Pump	Spare T-502 Pump
C-401	Process Machinery	$5,498,000	2.15	$11,821,000	Compressor	R-401 Recirculation Compressor
C-501	Process Machinery	$1,740,000	2.15	$3,740,000	Compressor	S-502 Compressor

Table 17.2 Equipment Cost of Fabricated Equipment

Unit ID	Purchase Cost ($)	Bare Module Factor	Bare Module Cost ($)	Unit Type	Description
E-101	$42,900	3.17	$135,800	Heat Exchanger	R-201 Feed HX
E-201	$33,200	3.17	$105,300	Heat Exchanger	R-201 Recirculation HX
E-303	$22,100	3.17	$70,200	Heat Exchanger	Trimers Stream HX
E-401	$586,300	3.17	$1,859,000	Heat Exchanger	R-401 Feed HX
E-503	$26,200	3.17	$83,100	Heat Exchanger	Xylene Stream HX
E-302	$26,800	3.17	$84,900	Heat Exchanger	Trimer Column Condenser
E-301	$43,900	3.17	$139,000	Heat Exchanger	Trimer Column Reboiler
E-502A	$108,000	3.17	$342,400	Heat Exchanger	Xylene Column Condenser A
E-502B	$108,000	3.17	$342,400	Heat Exchanger	Xylene Column Condenser B
E-501	$31,900	3.17	$101,100	Heat Exchanger	Xylene Column Reboiler
E-C501A	$12,100	3.17	$38,400	Heat Exchanger	C-501 Intercooler A
E-C501B	$12,500	3.17	$39,800	Heat Exchanger	C-501 Intercooler B
E-504	$22,100	3.17	$70,100	Heat Exchanger	S-502 Feed HX
E-402	$1,084,000	2.19	$2,373,000.00	Furnace	R-401 Recirculation Furnace
R-201	$384,400	4.16	$1,600,000	Reactor	Oligomerization Reactor
R-401	$432,200	4.16	$1,798,000	Reactor	Dehydrocyclization Reactor A
R-402	$432,200	4.16	$1,798,000	Reactor	Dehydrocyclization Reactor B
R-403	$432,200	4.16	$1,798,000	Reactor	Dehydrocyclization Reactor C
R-404	$432,200	4.16	$1,798,000	Reactor	Dehydrocyclization Reactor D
S-301	$150,000	4.16	$785,200	Distillation Column	Trimer Separation Dist. Column
S-501	$300,000	4.16	$1,793,000	Distillation Column	Xylene Separation Dist. Column
S-502	$9,600	4.16	$39,900	Flash Drum	Hydrogen Separation Flash Drum
D-301	$36,300	4.16	$163,400	Drum	Trimer Column Reflux Accumulator
D-501	$59,400	4.16	$247,200	Drum	Xylene Column Reflux Accumulator

All equipment costs were calculated using the Equipment Cost Spreadsheet provided by the Penn professors. Standard cost equations are used in the spreadsheet.[24] Because the cost equations are based on prices in mid 2014, a CE Index of 644.3 was calculated for 2020, the year our project is halfway finished with spending money on construction. Tables 17.1 and 17.2 above show the purchase costs and bare module costs of the equipment in the plant. The storage equipment includes both storage tanks and surge tanks, process machinery includes pumps, and fabricated equipment includes heat exchangers, a furnace, reactors, separators, and drums. The total cost of all of the equipment is \$40.6 MM. The total cost of spares is \$1.01 MM. Spares were bought for all pumps. Figure 17.1 shows the breakdown of the costs.

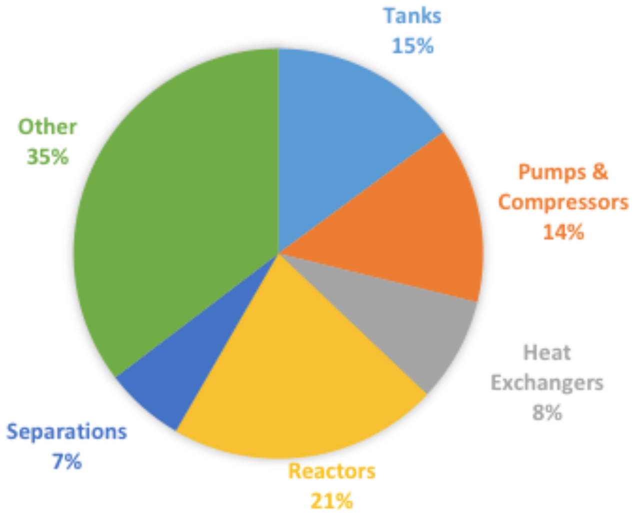


Figure 17.1 Pie chart showing what percentage each type of equipment is of the total cost, \$40.6 MM.

As shown in the figure, the “Other” section, which includes the blower in the R-401 recirculation loop, accounts for over one third of the total cost of equipment. Reactors account for just less than one fifth, storage/surge tanks and pumps/compressors are slightly less than that, and heat exchangers and separators account for the rest. The tanks and pumps account for a large amount of the price due to the large quanitity of these pieces of equipment needed. Additionally, the storage tanks are expensive due to their large volume because of the large flow rate of the plant.

The most expensive piece of equipment, by far, is the centrifugal turbo blower in the recirculation loop around R-401. The purchase cost is $5.50 MM, and the bare module cost is $11.8 MM. This piece of equipment is very expensive due to its large size, which processes 1.40 MM lb/hr of material. The material is stainless steel due to the high temperature of the fluid, making the piece of equipment much more expensive.

Ignoring the "other" category of equipment, it was expected for reactors to account for the largest percentage out of all of the equipment. R-201 costs $1.6 MM, due to the large flow rate and large mass of catalyst in the reactor. R-401 consists of four reactors that each cost $1.80 MM, for a total cost of $7.20 MM. This reactor is very large due to the large recirculation flow rate to improve the low conversion and the large amount of catalyst due to the low WHSV. Furthermore, the reactors have to be made of stainless steel 304 because they are running at high temperature, and this greatly increases the cost.

Other expensive pieces of equipment to note above $1 MM include the compressor C-501, the heat exchanger E-401, the fired heater E-402, and the distillation column S-501. The compressor before the flash is expensive because it is compressing a large amount of material from 24 psig to 285 psig, which requires three stages and a large amount of horsepower. The heat exchanger E-401 is expensive because it involves very large temperature differences: one stream must reach the inlet temperature of R-401, which is very high, and another stream leaves R-401 to enter a separation column. This creates a large surface area. Additionally, this heat exchanger has to be made of stainless steel 304 due to its high temperature, which increases the price greatly. Fired heaters are generally capital-intesive due to their high temperature, so it was expected for this to have a high cost. Lastly, the distillation column S-501 has three exit streams. The large inlet stream needs to be separated very well to obtain a stream that is 89 wt% p-xylene, a stream containing the materials in the process to recycle, and a stream that is mostly hydrogen. This requires many trays, making the column very tall and expensive.

Section 18
Fixed Capital Investment Summary

The Profitability Analysis Spreadsheet provided by the UPenn professors of CBE460 was used to model financials. While the plant will have a 30-year lifetime, the financials are modeled over 10 years because it is unreliable to forecast any farther out.

Section 18.1 Equipment and Catalysts Costs

The total bare module costs include all equipment and catalysts. After determining the bare module costs for the necessary equipment, the total capital investment was assessed with the recommended methods[24]. The total equipment purchase cost required for the design is \$72.7 MM. \$40.6 MM of this is cost of the equipment, and a more detailed breakdown of these costs is in Section 17.

The catalysts are also included in the initial purchasing cost for necessary equipment; \$32.1 MM accounts for the cost of the two catalysts. The pricing breakdown is shown in Table 18.1 below. The price of HZSM-5 is \$20.00/lb, with a total cost of \$1.44 MM.[10] For both catalysts, a bare module factor of 1.5 was used, decided on by assessing freight costs for different order sizes and the labor necessary to install the catalysts into the reactors. Therefore, the total bare module cost for HZSM-5 is \$2.16 MM. New catalyst will need to be bought throughout the plant lifetime. When needed, a purchase order will be placed.

The price of the Cr/Al_2O_3 catalyst was calculated based on discussions with consultants.[10] The patent specifically mentioned a catalyst from BASF, and it is assumed that the catalyst has 95% alumina. We were told that the cost of the catalyst is heavily dependent on the metal cost and that the cost of alumina is \$7.00/lb. The cost of chromium is less expensive at \$3.50/lb. An additional loading cost should be added in, but due to the lack of data, we are assuming this cost is negligible. Furthermore, the total catalyst lifetime of Cr/Al_2O_3, even with regeneration, is assumed to be five years. Therefore, because the spreadsheet models the plant over ten years, the plant will require two purchase orders of the catalyst. Each purchase will cost \$10 MM. A bare module factor of 1.5 was used to obtain a total cost of \$30 MM for the two orders over the 10 years projected on the spreadsheet. Information on the amount of utilities and costs relevant to catalyst regeneration are detailed under operating costs in the Section 19.5.

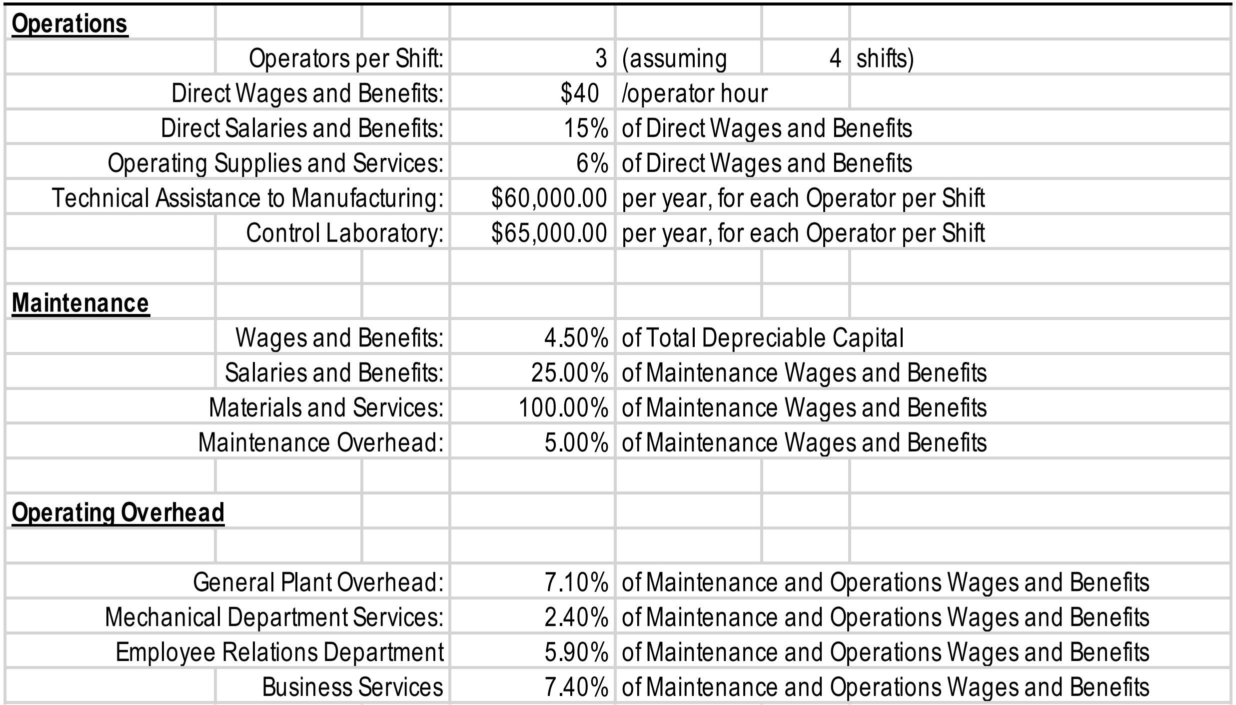
Table 18.1 Costs of the Two Catalysts. The amount of catalyst is how much will initially need to be bought. The 10-year cost assumes that the HZSM-5 was purchased once and the Cr/Al_2O_3 was purchased twice.

Material	**Cost per lb**	**Amount (lb)**	**Purchase Cost**	**Bare Module Factor**	**10-Year Cost**
HZSM-5	\$0.50	71,809	\$36,000	1.5	\$54,000
Cr/Al_2O_3 Catalyst Total	\$3.50/5% Cr \$7.00/95% Al	1.90 MM	\$20.0 MM	1.5	\$30.0 MM

Section 18.2 Operations, Maintenance, and Overhead

After determining the relevant equipment and catalyst costs, operations and maintenance were examined. Discussions with consultants indicated that a plant of this size would require 5 operators for startup, and 3 from the third year of production onward. Each operator would be responsible for one process area: the oligomerization process, the dehydrocyclization process, and the general storage and transfer of material throughout the process. There will be four shifts, which will allow a 40-hour work week with 8-hour shifts or 12-hour shifts. We will need 3 operators per shift and 1 laboratory per shift by the third year. The remaining values for operations, maintenance, and overhead defaulted to general recommendations, as there was no indication that this process would deviate from the scope of those heuristics.[24] All values are shown in Table 18.2 below.

Table 18.2 Operations, Maintenance, and Operating Overhead Inputs

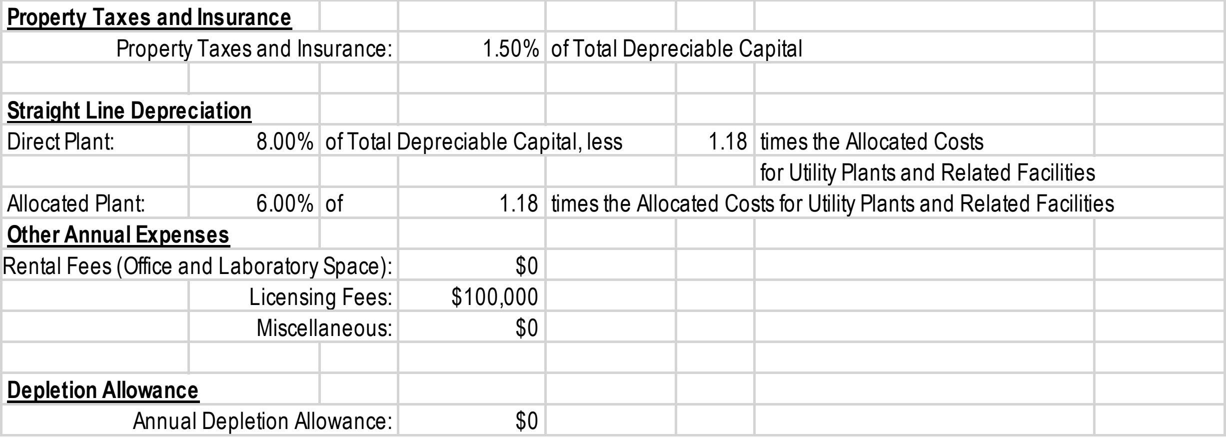


Operations				
Operators per Shift:	3	(assuming	4	shifts)
Direct Wages and Benefits:	$40	/operator hour		
Direct Salaries and Benefits:	15%	of Direct Wages and Benefits		
Operating Supplies and Services:	6%	of Direct Wages and Benefits		
Technical Assistance to Manufacturing:	$60,000.00	per year, for each Operator per Shift		
Control Laboratory:	$65,000.00	per year, for each Operator per Shift		
Maintenance				
Wages and Benefits:	4.50%	of Total Depreciable Capital		
Salaries and Benefits:	25.00%	of Maintenance Wages and Benefits		
Materials and Services:	100.00%	of Maintenance Wages and Benefits		
Maintenance Overhead:	5.00%	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		

Section 18.3 Other Fixed Costs

Property taxes and insurance were assumed to be 1.5% of the total depreciable capital, given the relatively sparse settling of the proposed site location in Iowa. Depreciation was calculated in accordance with the MACRS code. There are no expected rental fees or depletion allowances, but $100,000 is appropriated for licensing the patent information and associated research from GEVO, so as to better model and control the process.

Table 18.3 Insurance and Other Fixed Costs



Property Taxes and Insurance				
Property Taxes and Insurance:		1.50%	of Total Depreciable Capital	
Straight Line Depreciation				
Direct Plant:	8.00%	of Total Depreciable Capital, less	1.18	times the Allocated Costs
				for Utility Plants and Related Facilities
Allocated Plant:	6.00%	of	1.18	times the Allocated Costs for Utility Plants and Related Facilities
Other Annual Expenses				
Rental Fees (Office and Laboratory Space):		$0		
Licensing Fees:		$100,000		
Miscellaneous:		$0		
Depletion Allowance				
Annual Depletion Allowance:		$0		

Section 18.4 Total Permanent Investment

Along with the costs above, there will be fees associated with building the plant. These fees are stated in Table 18.3. These were defaulted to general recommendations.[24]

Table 18.4 Fees and their percentages of the costs

Investment Summary Specifics	**Percentages**
Cost of Site Preparations	5% of Total Bare Module Costs
Cost of Service Facilities	5% of Total Bare Module Costs
Allocated Costs for utility plants and related facilities	$0
Cost of Contingencies and Contractor Fees	23% of Direct Permanent Investment
Cost of Land	2% of Total Depreciable Cost
Cost of Royalties	$0
Cost of Plant Start-Up	15% of Total Depreciable Capital

Section 18.5 Investment Summary

Table 18.5 below shows the actual costs calculated by the spreadsheet. This table shows that we will need a total permanent investment of $100.4 MM.

Table 18.5 Total Permanent Investment

Investment Summary			
Total Bare Module Costs:			
Fabricated Equipment	$	16,885,862	
Process Machinery	$	-	
Spares	$	-	
Storage	$	6,147,948	
Other Equipment	$	-	
Catalysts	$	32,124,996	
Computers, Software, Etc.	$	-	
Total Bare Module Costs:			**$ 55,158,806**
Direct Permanent Investment			
Cost of Site Preparations:	$	2,757,940	
Cost of Service Facilities:	$	2,757,940	
Allocated Costs for utility plants and related facilities:	$	-	
Direct Permanent Investment			**$ 60,674,687**
Total Depreciable Capital			
Cost of Contingencies & Contractor Fees	$	13,955,178	
Total Depreciable Capital			**$ 74,629,865**

Table 18.5 (continued) Total Permanent Investment

Total Permanent Investment				
Cost of Land:	$	1,492,597		
Cost of Royalties:	$	-		
Cost of Plant Start-Up:	$	11,194,480		
Total Permanent Investment - Unadjusted			$	87,316,942
Site Factor				1.15
Total Permanent Investment			**$**	**100,414,483**

Section 19
Operating Cost

Section 19.1 Raw Materials

The principle feedstock for this process is the sustainably-source isobutylene. Per the project statement, it can be secured over the project's lifespan for 90% of its market price. The cost of isobutylene was determined from the ICIS database to be about \$0.81/lb, so we can purchase it for \$0.75/lb.[18] The process also requires a small stream of isooctane to make up for diluent lost on each cycle, which costs \$0.17/lb and is relatively less significant to the financials.[11] Ratios of the amount of raw material used per amount of product made were calculated from the design process and input into the profitability analysis spreadsheet, as shown below.

Table 19.1 Cost of two main raw materials

Raw Material	Ratio (lb per lb of product)	Cost (per lb)	Yearly Requirement (lb)	Annual Cost
Isobutylene	1.597	\$0.75	1.0 B	\$730 MM
Isooctane	0.006	\$0.17	3.5 MM	\$596 M

Although commodity chemical prices are not expected to be stable long-term, the price of isobutylene is set by our internal supplier and is modeled as increasing with general inflation. Factors that drive the price of isobutylene, especially on the demand side, also impact the price of p-xylene, so there is more uncertainty in exact pricing than there is on the process's spread.

Section 19.2 Utilities

Following the calculations from Section 14, the yearly utility requirements were determined from the necessary flowrates. Where possible, standard prices were used for the relevant costs.[24] These costs are tabulated below in Table 19.2 and are not expected to vary significantly over the lifespan of the project. Although it may prove less profitable, we recommend further exploration of sustainably sourcing these utilities, as the added environmental friendliness would increase the "green value" of the product and potentially make it easier to secure a higher premium for the p-xylene.

Table 19.2 Utility Cost. The only utility missing is air. We assume the cost of this is negligible and that our company's plant already has an air supply.

Utility	Ratio (lb or kWh per lb of product)	Cost (per lb or kWh)	Yearly Requirement (MM of lb or kWh)	Annual Cost ($MM)
150 psig Steam	0.709	$0.007	554 MM	$3.88
1250 psig Steam	2.173	$0.011	1.36 B	$15.0
Cooling Water	51.28	$0.000012	32.0 B	$0.39
Chilled Water	31.62	$0.00031	11.0 B	$3.81
Nitrogen	0.148	$0.01	449 MM	$0.93
Natural Gas (Methane)	0.0007	$0.12	11 MM	$1.33
Refrigeration	0.0006	$0.00004	19.4 MM	$0.778
Electricity	0.136 kWh	$0.70	21.1 MM	$14.8

Section 19.3 Variable Costs

Figures for other relevant variable costs were sourced from standard guidelines, with the default recommendations used for most values.[24] However, due to the high-cost small-margin nature of the venture, these costs were fixed to the earnings rather than the sales of the project. These values are back-calculated as a percentage of sales to give the correct values, so they do not correspond to the values entered in the spreadsheet due to limitations in editing the spreadsheet.

Table 19.3 General Expenses

General Expenses	Percentage of Sales (%)	Annual Cost ($MM)
Selling / Transfer Expenses	3.00	28.1
Direct Research	3.00	28.1
Allocated Research	0.10	0.94
Administrative Expense	2.00	18.7
Management Incentive Compensation	1.25	11.7
Total	9.35	87.7

Including the raw materials, byproducts, and utilities with general expenses, the total variable cost for plant operation is $874 MM.

Section 19.4 Fixed Costs

The percentages used for calculating fixed costs are shown in Tables 19.2 and 19.3. The costs calculated are shown in Table 19.4 below. The total fixed cost of plant operation is $12.5 MM.

Table 19.4 Breakdown of fixed costs from Profitability Analysis spreadsheet

Operations			
	Direct Wages and Benefits	$	998,400
	Direct Salaries and Benefits	$	149,760
	Operating Supplies and Services	$	59,904
	Technical Assistance to Manufacturing	$	720,000
	Control Laboratory	$	780,000
	Total Operations	**$**	**2,708,064**
Maintenance			
	Wages and Benefits	$	3,247,394
	Salaries and Benefits	$	811,848
	Materials and Services	$	3,247,394
	Maintenance Overhead	$	162,370
	Total Maintenance	**$**	**7,469,005**
Operating Overhead			
	General Plant Overhead:	$	369,726
	Mechanical Department Services:	$	124,978
	Employee Relations Department:	$	307,237
	Business Services:	$	385,348
	Total Operating Overhead	**$**	**1,187,288**
Property Taxes and Insurance			
	Property Taxes and Insurance:	$	1,082,465
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	$	-
	Licensing Fees:	$	100,000
	Miscellaneous:	$	-
	Total Other Annual Expenses	**$**	**100,000**
Total Fixed Costs		**$**	**12,546,822**

Section 19.5 Catalyst and Regeneration Process

Operating costs for catalyst regeneration were included in the bare module factor. As stated previously, the HZSM-5 catalyst must be regenerated every year, and the Cr/Al catalyst must be regenerated every five days in an eight-hour controlled burn. To calculate the amount of utilities needed for the decoking process, the 7% coke rate was used with the catalyst mass to estimate the coke deposit. This was then used to calculate the oxygen flow-rates necessary for regeneration. A 1% oxygen stream is creating by feeding nitrogen and air into the system, as explained in Section 13.4.2. This amounts to 93 MM pounds of nitrogen per year and 43 MM pounds of air per year, as shown in the calculations in the Appendix in Section 25.3.7. These utility costs are included in Table 19.2.

Section 20
Profitability Analysis

Section 20.1 Analysis of Two Business Cases

The profitability of the proposed process design and product yield is evaluated under two cases. First, we consider the expected return if the p-xylene was to be sold at its current price in today's markets. We then consider the premium necessary to yield a 15% investor's rate of return.

Case A: Current Market Prices

From ICIS, the market price of p-xylene has fluctuated over the last year between \$0.55 and \$0.80 per lb. Further research into crude pricing indicated that the largest factor was purity. Given the 89% purity of the product, the price estimate was placed at \$0.75 per lb, and set to grow with general inflation, due to the lack of detailed pricing predictions available. This price also includes the \$10/ton cost the third-party separator will charge for purifying the final xylene stream into p-xylene.

Unassisted by a premium, this project is financially unattractive, which was expected. The investor's rate of return is negative, and the net present value of the project is a loss of \$1.01 B. Though discouraging, this is due to fundamental economic potential - even with a 10% discount on the isobutylene, the process requires 1.6 lb of it for every lb of product produced, costing \$1.15 per lb of product. This limit means that any p-xylene price below that threshold of \$1.15 is decidedly unprofitable, regardless of internal efficiency improvements. Given the nature of this business case, it is not examined in depth, but all calculations and sensitivities pertinent to the second case are unchanged.

Table 20.1 Summary of Profitability Measurements for Case A

Profitability Measure	**Amount** **IRR & ROI (%)** **Profit ($)**
IRR	Negative IRR
NPV in 2018	(1.04) MM
ROI Analysis (3rd Production Year)	
Annual sales	489 MM
Annual Costs	(803) MM
Depreciation	(8.03) MM
Income Tax	(77.4) MM
Net Earnings	(245) MM
Total Capital Investment	117 MM
ROI	-210%

Case B: Pricing Premium

Per request, we also examined the business case where a green pricing premium could be levied on the p-xylene. After the rigorous profitability calculations were tabulated in the spreadsheet, Excel's GoalSeek feature was used to determine the premium that would yield a 15% IRR on the project. A premium of 79%, increasing the price to $1.35/lb, was found to yield a 15.01% return.

Table 20.2 Summary of Profitability Measurements for Case B

Profitability Measure	**Amount** **IRR & ROI (%)** **Profit ($)**
IRR	15.01%
NPV in 2018	40.3 M
ROI Analysis (3rd Production Year)	
Annual sales	877 MM
Annual Costs	(839) MM
Depreciation	(8.03) MM
Income Tax	(7.07) MM
Net Earnings	22.4 MM
Total Capital Investment	155 MM
ROI	14.48%

The Net Present Value of this business case was calculated to be $40,300, but this number should be contextualized. Spreadsheet limitations constrain the project's lifespan to 20 years, and consultants informed us of the dangers of predicting too far into the commodities markets. With that in mind, the return is set to 15% after 10 years of production, which marks 13 years from the beginning of project design. Because the equipment, spares, and regeneration are included for a plant that can operate for 30 years after construction is completed, possible projected returns were found. Extending the project beyond this milestone does not change the IRR dramatically (up to 18% for 20 years), but does increase the net present value, as working capital was exhausted in Year 3 and all equipment has been fully depreciated by Year 7, meaning that all years thereafter are more focused on production. Figure 21.1 tracks the projected IRR and NPV for the years of production that extend beyond the modeled 10-year lifespan.

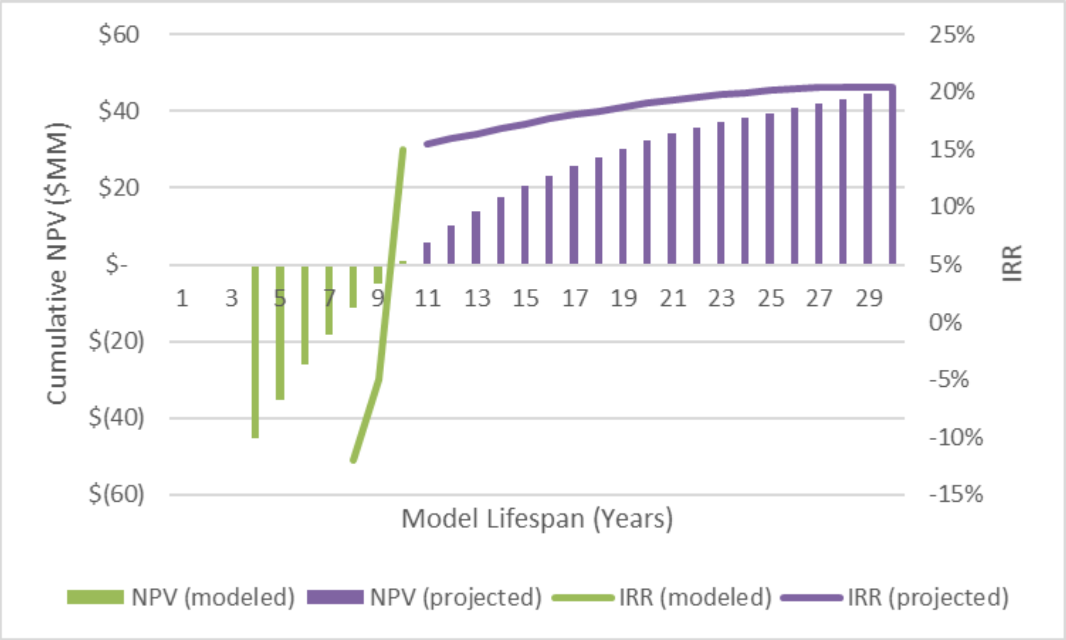


Figure 21.1 Modeled and projected profitability measures over the lifespan of the project

As seen in Figure 21.2, the profitability of the project is very sensitive to the price premium on p-xylene. Though a 79% premium is sufficient to secure a 15% return, negotiating a slightly higher price would greatly increase the profitability. Increasing from the base case of $1.35 to $1.37

per lb, for example, which only raises the premium to 81%, raises the projected IRR to 21%. These added returns could be used to defray the large permanent investment necessary for the project.

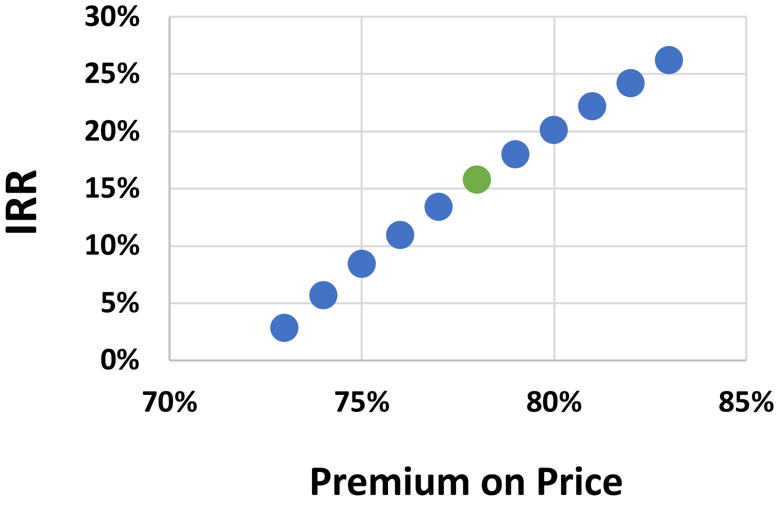


Figure 21.2: Sensitivity of return to p-xylene price premium

Section 20.2: Analysis of Profits from Trimers

As the trimer stream is produced at about half the production rate of p-xylene, its price is also a sensitive factor to the project's profitability. The price estimate, based off the composition of the stream, current sales rates, and correspondence with Honeywell, should be examined at different values to understand how the coproduct's price impacts the project's profitability. As shown in Figure 21.3, a modest increase in the price of the trimer stream would drive a considerable increase in returns. Given that there are increasingly more financial incentives for green products in the commodity chemical industry, as discussed in Section 4, these opportunities should be explored further to increase the project's profitability.

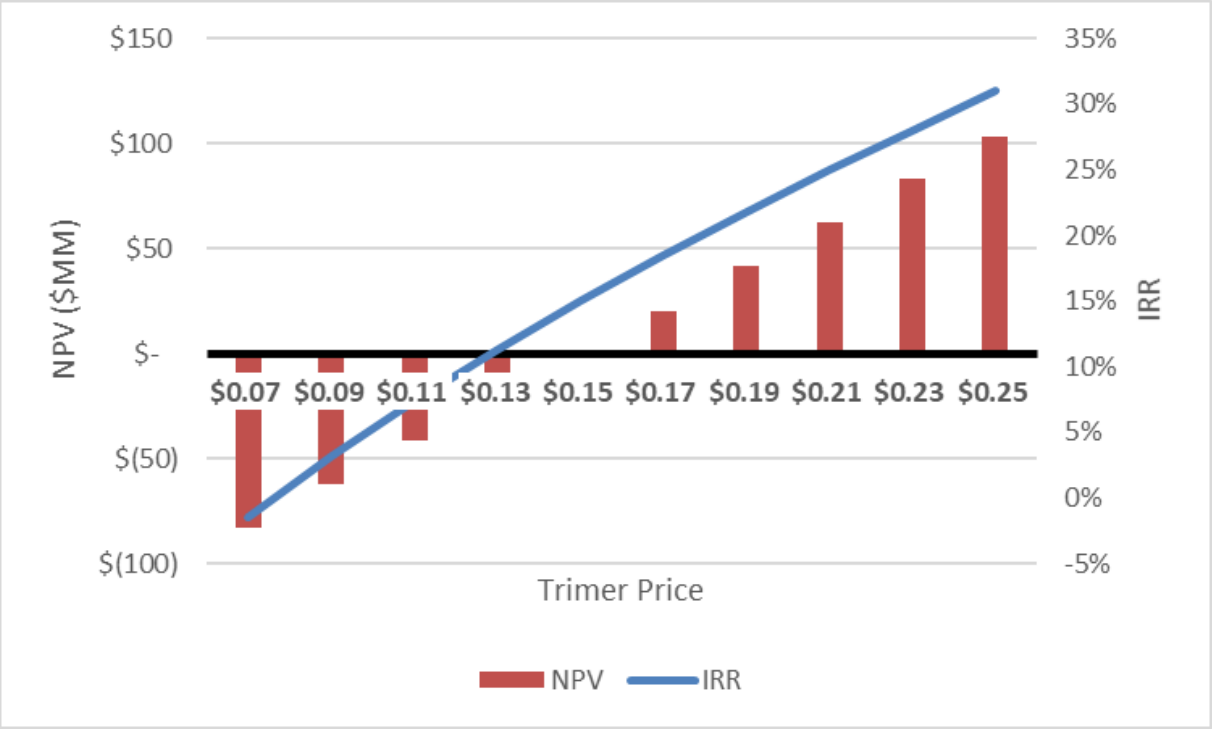


Figure 21.3: Sensitivity of profitability measures to price of trimers stream

Section 21

Other Important Considerations

Section 21.1 Environmental

The plant will be located in Iowa due to the state's access to sustainable raw material and because xylene separation plants are located here, as previously stated. It will also be next to the Mississippi River so that equipment can be efficiently delivered via waterway. As a result, more precautions must be taken to avoid contaminating the water and harming humans and animals. Isooctane is fatal to marine life, and its detrimental effects last for a long time according to its safety data sheet. Similarly, TMP and trimers are also lethal to aquatic life. Safety analysis done on all chemicals shows that no corrosive materials are involved in the plant, reducing the potential of pipe leakage. More thorough investigations on leakage prevention and waste management were performed. Products of the plant are stored in storage tanks, and the only gas exhaust in this system is fed into the fired heater. Apart from these precautions, this plant will adhere to environmental policies established by the United States Environmental Protection Agency (EPA) such as the Clean Air Act, Clean Water Act, and the Pollution Prevention Act to mitigate environmental contamination.

Section 21.2 Process Control and Instrumentation

The plant will employ a typical control system of a hydrocarbon plant. The system should either ensure that the pressures and temperatures of streams and equipment are at acceptable conditions by modifying certain aspects or notify operators if there are issues. In particular, there should be instrumentation associated with oxygen leaks. Because most of the chemicals are flammable, extensive oxygen level checks will be performed throughout the plant and in storage tanks. Isooctane and p-xylene, in particular, are incredibly reactive with oxygen, so the MSDS sheets recommend that the minimum oxygen level be maintained at 29% by volume. While oxygen level checks must occur constantly, they should especially occur after decoking R-401, where oxygen is introduced to the system through an air feed.

Section 21.3 Safety and Health

Due to the use and formation of different hydrocarbons in the design, fire hazards are a primary concern. TMP, p-xylene, trimers, and isobutylene are very flammable, so the instrumentation that detects oxygen leaks will help avoid explosions. Nitrogen blankets should be installed on storage and surge tanks that do not have a floating head. The tanks will not be full, creating a headspace for oxygen. Nitrogen in the headspace maintains a safe oxygen concentration in the tank, preventing an explosion.

Additionally, inhaling TMP and xylene can cause severe lung damage, and vaporized isooctane can also displace oxygen and cause asphyxiation. For these reasons, all leaks must be immediately identified and fixed. Having physical contact with any of the hydrocarbons used can cause extreme irritation, so plant personnel will be required to wear PPE, such as hand protection, body protection, eye protection, and flame-resistant gear at all times on site. Those working directly with the chemicals will also be required to wear respiratory protection. Guidelines by the National Institute of Occupational Safety and Health (NIOSH) will be followed.

Section 21.4 Startup

The main differences in start-up is the amount of material entering the system. As the process runs, only the amount of isooctane (the diluent) lost in the exit streams needs to be made-up. To inventory the plant, the amount of isooctane added should be 10% of the total hourly flow rate. This equates to about 100,000 pounds. This initial amount will need to be added after the annual shutdown and after any unexpected shutdowns.

Additionally, oxygen levels are a main concern at startup. According to MSDS in Section 25.5, the oxygen levels should not exceed 19.5% by volume. Therefore, if the amount detected is above this level, pure nitrogen will be used to flush the system before starting the operation. Three times the total volume of the equipment worth of nitrogen should be used in this process, with an additional half of the total volume to take into account the lengths of the pipes.

Lastly, as stated in Section 15.1, the pumps will have a larger flow rate of fluid flowing through them during start-up.

Section 21.5 Other Considerations

Because the two reactors operate at different phases, our plant must adequately handle both vapor and liquid components. Phase changes are not desired in equipment other than separators to avoid flashing. The only time flashing is expected is when the liquid overhead from the trimer distillation column enters E-401. To avoid unwanted flashing elsewhere, the pressure of liquid streams will be increased before getting heated by heat exchangers. For example, the inlet stream should be increased all the way to 50 psig for safety. NRTL is used to model every component, but additional research on the specific components within the plants and how they interact should be done to avoid flash points when needed.

Trimer selection should be better considered. While we chose 1-dodecene, it was later suggested that the choice of trimer should be a conservative assumption, meaning the trimer should have a boiling point close to the compound it is being separated from. This would ensure the boiling point difference in actuality is larger than what ASPEN thinks it is, creating a conservative estimate.

TMP has a boiling point of 212ºF. 1-dodecene has a boiling point of 415ºF, while most trimers have a boiling point of 265ºF. Therefore, 1-dodecene is not the optimal choice because its boiling point temperature difference with TMP is larger than most trimers. This should not affect the current process and results greatly because the boiling point difference between most trimers and TMP is 53ºF, which is still a large amount. If a conservative assumption were to be made instead, the trimer used should be 1-undecene, which has a boiling point of 376ºF, a value close to most trimers. It was suggested that if we use 1-dodecene, we should increase the column height by adding three trays to cover any uncertainty. Equipment design and operations would be slightly different if the trimer were changed or if the column height were increased.

Another design specification that should be followed for columns is to not exceed a bottoms temperature of 450ºF. This is important to prevent polymerization. While the bottoms temperature of S-501 is within range at 367ºF, the bottoms temperature of S-301 is at 543ºF, which is too high. The amount leaving the top of the column should be increased to decrease the bottoms temperature.

Lastly, it is important to note that our final stream purity is 89 wt% p-xylene, and the problem statement asked for 90 wt% p-xylene. In the problem statement, we were given a cost to separate a xylene stream that is 90 wt% p-xylene. Because 89 wt% is very close to 90 wt%, this cost did not change. While we did our best to optimize the process, there is room for improvement. If we were to optimize further, we would focus on the separation columns because the reactor conditions are already set by the patent, and we do not have kinetics information. It is difficult to accurately model this process without kinetic data, so obtaining this information is vital.

Section 21.6 Plant layout

Federal, state, and OSHA regulations are considered when designing the plant. Figure 21.1 shows the preliminary layout of the plant. Storage tanks for isooctane, isobutylene, trimers, and p-xylene will be kept in a tank farm in one section of the plant. The process area will be next to the tank farm, which includes all operating equipment. Offices and the maintenance workshop are located near the plant for workers' convenience.

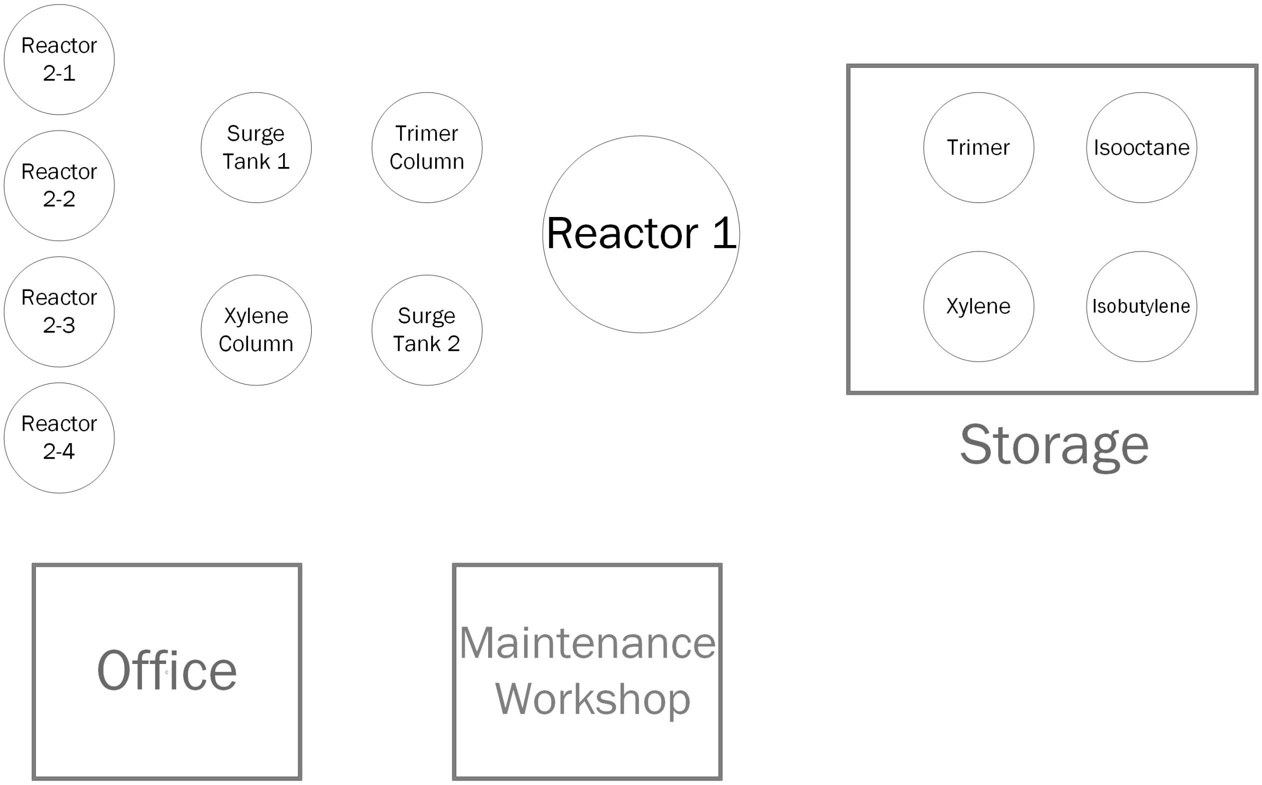


Figure 21.1: Preliminary layout for the plant

Section 22
Conclusions and Recommendations

To secure an investor's rate of return of 15% on the sustainable product, a premium of 79% over p-xylene's market price is required. Given the cost-sensitive nature of the commodities market, we do not recommend proceeding before further investigating the long-term value. In the context of textile manufacturers marketing their products as sustainable, this process offers a key intermediate step to green plastic fibers. While the process design for isobutylene to p-xylene shows promise of an attractive return, without detailed information on the external steps of the process, such as the intermediaries to PET, the premium necessary is too high to confidently expect to meet demand at that price.

Should the process be revisited, the estimate for the premium could be confidently lowered with more data. The process design in this report states a few assumptions and lacks necessary data that must be further researched and explored before fully evaluating the success of creating the manufacturing plant. First, there is very limited data on the Cr/Al_2O_3 catalyst, so detailed kinetic and thermodynamic research on the catalytic pathways would augment experiment design and the usefulness of ASPEN's analysis. While the patent states a lifetime of only 15 minutes, industry professionals and other journal articles state that the catalyst lasts 5 days, which is what was used in this report. Additional laboratory experiments on catalyst lifetime must occur. Furthermore, the length of the decoking process was obtained from journal articles, but many had conflicting data. Further research and additional laboratory experiments should be done on this as well. With this research, the equipment design would be improved with a step-by-step cost-benefit analysis. Another assumption made was the choice of diluent. Isooctane was chosen based on data throughout the patent, but the examples from the pilot plant do not include isooctane. More research should be done analyzing if isooctane is the best diluent and what exactly is the role of isooctane: simply kinetics or also thermodynamics. Lastly, assumptions were made with regard to the reactors.

Recirculation loops were added to increase conversion, and while the patent does not mention the reactions being equilibrium-limited, this should be tested. Along with these assumptions, all design calculations done in Appendix Section 25.3 and explained in Section 15 should be reviewed by a professional engineer, along with the energy and utilities requirements in Section 14. Assumptions made in this report about demand for sustainable products and the lack of widely-used environmental certifications should be updated given the quickly-changing nature of the green market.

While the delivered estimate for the premium of 79% is not yet attractive, this design report uses the available resources to intelligently reduce uncertainty, confidently banding that to 79 ± 20%. Drawing from theory in several fields of chemical engineering, research into existing patents, designs, and operations, and consultancy with distinguished experts in relevant practices, we aim to provide certainty wherever feasible and recognize the boundaries of this projects scope. Although we do not recommend immediate construction and stress verification and updates to the calculations as necessary, we are confident that this process design will one day be profitable, feasible, sustainable, and useful. Consumers are moving toward buying green clothes, and clothing manufacturers use textiles, and textile producers rely on plastics. A sustainable product must originate from a sustainable plastic. The missing link, available at a considerable premium, is p-xylene from biomass.

Section 23. Acknowledgement

We could not have completed this project without the help of many people whom we would we like to thank here. Thank you to Dr. Holleran and Professor Vrana for their guidance each week and for keeping us moving forward in the right direction. We would also like to thank Dr. Bockrath for proposing this project and quickly helping us navigate key decisions. The consultants who joined us offered vast knowledge, especially Mr. Sawyer and Mr. Brostow. Additionally, thank you to Dr. Gorte for helping us with knowledge on catalysts and reactor design. Lastly, we would like to give a huge thank you to Professor Fabiano, who helped us tremendously with our ASPEN flowsheet and process design.

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Section 25
Appendix

Section 25.1
Project Problem Statement

1. Process for Sustainably Sourced p-Xylene
(recommended by Rick Bockrath, Consultant - formerly DuPont)

Problem Statement

You work for a biotechnology company that has a supply of isobutene produced from biomass. Your company is interested in converting this sustainably sourced isobutene to higher value products. You are part of a team tasked to develop a plant design and economic estimates for a para-xylene facility based on recent patents and other technical literature. The ultimate product is PET for fibers. At this point it is believed that PET bottles cannot "afford" the required pricing premium. The other part of the PET polymer is based on ethylene glycol. Producers in Brazil have apparently successfully started up commercial scale EG plants based on ethanol and are able to command a significant price premium over petrochemical EG (100%) for select markets. Your marketing organization is optimistic that the fibers segment can accept the needed upcharge. Your focus is on defining the magnitude of the needed premium to make the venture profitable.

Background

In 2014, global para-xylene demand was estimated at 36.83 million tons and is estimated to exceed 62.98 million tons at a CAGR of 7.0% from 2015 to 2022. This growth is due to increasing demand for fiber and polyester resin in numerous end-use applications across various industries. Growing utilization of purified terephthalic acid (PTA) for polyester production, particularly in Asia Pacific is expected to fuel growth in paraxylene market over the forecast period. Rising demand for bio-based alternatives and increasing consumer awareness subject to non-biodegradable nature of petrochemical products is expected to be the major obstacles for market participants. A sustainably sourced alternative may have a market advantage even at a price premium. The current market price for para-xylene is about $700 - $800/metric tonne.

In petrochemical processing, xylenes are produced via catalytic reforming. A low octane naphtha cut (typically a straight run or hydrocracked naphtha) is converted into high-octane aromatics, including, benzene, toluene, and mixed xylenes. The amount of xylenes contained in the catalytic reformate depends on the fraction and type of crude oil, the reformer operating conditions, and the catalyst used. The amount of xylenes produced can vary widely, typically ranging from 18 to 33 vol % of the reformate. The unrecovered reformate xylenes are used in the gasoline pool.

The mixed xylenes that are recovered from these sources are used as follows: 50 – 60% to make PX, 10 – 15% to make OX, 10 – 25% returned back to gasoline blending, and only 1% to make MX. The relative lack of end uses for MX is unfortunate, because the catalytic reformate sources typically contain twice as much MX as PX or OX. The majority of the MX in these sources is isomerized to PX and OX. The purified xylenes are used to synthesize plasticizers and polyester fibers, photographic films, and beverage bottles. PX is first oxidized to terephthalic acid or dimethyl terephthalate before being converted into polyesters. OX is oxidized to phthalic anhydride before being converted into plasticizers. MX is oxidized to isophthalic acid, which is used to make polyesters.

GEVO Process from Isobutanol

Your team has performed a detailed patent review of various processes and a clear conclusion is that isobutene to xylene catalysts are known to be prone to coking and low conversion. Recent patents from GEVO have outlined a route to relatively high purity p-xylene through careful selection of catalysts and

process conditions. A key difference in their patent is that the olefin to aromatic conversion step is done via the dimer of isobutene, isooctene. The IBN is converted to the dimer is a different reactor. The GEVO patent starts with isobutanol produced from fermentation. The isobutanol is dehydrated to isobutylene.

The isobutylene is then oligomerized, preferably to the dimer, and then undergoes a dehydrocyclization to form xylenes. Unconverted feed can be separated from the product of each reaction step and recycled. It may be necessary to add diluent in addition to this recycle in order to optimize the reaction step conditions.

Design Basis and Processing Alternatives

Your company produces isobutylene from fermentation, and you have 500,000 metric tonnes of isobutylene available as feed for your p-xylene facility. For the purposes of this study, you will use 90% of the nominal market price as your isobutylene transfer price. An October, 2016 report by Grand View Research indicates that 2015 pricing was $1740/met. tonne and that this will rise to $1900/met. tonne by 2024. You have been tasked along with your team to adopt the GEVO patent, along with other relevant technical literature, to design a facility to convert isobutylene to p-xylene.

You will need to determine the best reaction parameters for each step of the process. These are energetic reactions; you will need to decide whether additional diluents are needed to optimize the process conditions. Since there are multiple reaction steps, you should explore various configurations of the facility to determine the most economic design. Depending on your yields and selectivities, you will need to design a purification system(s) to recycle unreacted feed components and to obtain a xylene fraction. Your research has indicated that the required p-xylene purity must be greater than 99.7 wt% to be used as a polymer grade terephthalic acid process feedstock. While the patent gives examples with selectivity in excess of 99%, it is not clear that you can achieve the required 99.7 wt% routinely over the life of the catalyst. Therefore, for purposes of this study assume that you will generate a xylene “crude” product that is 90+ wt% p-xylene. The rest would be meta and ortho-xylene. This material will then be sent to an existing xylene separation plant, which is owned by another company, where the pure isomers will be recovered. Assume that the separator will charge you $50/metric tonne of xylene processed to separate the isomers.

The dehydrocyclization catalysts are known to be prone to coking of the catalyst. The catalyst fouling will ultimately stop the reaction. You will need to explore options for catalyst regeneration to enable an operational design. At this early stage of the design, the dehydrocyclization catalyst life has not yet been determined. You have been asked to develop the sensitivity of the process economics as a function of catalyst life.

At this scale and with IBN as the feedstock, it is expected that biobased p-xylene will not be cost competitive with petrochemical p-xylene. Therefore, a pricing premium will be required. You are to determine what market premium or subsidy is needed to have your p-xylene market competitive. Your company requires a minimum 15% IRR on this venture to move forward. The marketing organization would like you to “bracket” the needed premium. Therefore you are to study two cases;

a) The IRR and NPV for a case where the p-xylene is sold at current market prices.

b) A 15% IRR case where the pricing premium is included. The marketing organization wants to know the magnitude of the premium and the resulting projects NPV.

Section 25.2
Patent

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(54) **INTEGRATED PROCESS TO SELECTIVELY CONVERT RENEWABLE ISOBUTANOL TO P-XYLENE**

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(52) **U.S. Cl.** **528/308.3**; 585/240; 562/412

(57) **ABSTRACT**

The present invention is directed to a method for preparing renewable and relatively high purity p-xylene from biomass. For example, biomass treated to provide a fermentation feedstock is fermented with a microorganism capable of producing a C_4 alcohol such as isobutanol, then sequentially dehydrating the isobutanol in the presence of a dehydration catalyst to provide a C_4 alkene such as isobutylene, dimerizing the C_4 alkene to a form one or more C_8 alkenes such as 2,4,4-trimethylpentenes or 2,5-dimethylhexene, then dehydrocyclizing the C_8 alkenes in the presence of a dehydrocyclization catalyst to selectively form renewable p-xylene in high overall yield. The p-xylene can then be oxidized to form terephthalic acid or terephthalate esters.

Process for Preparing p-Xylene from Isobutanol

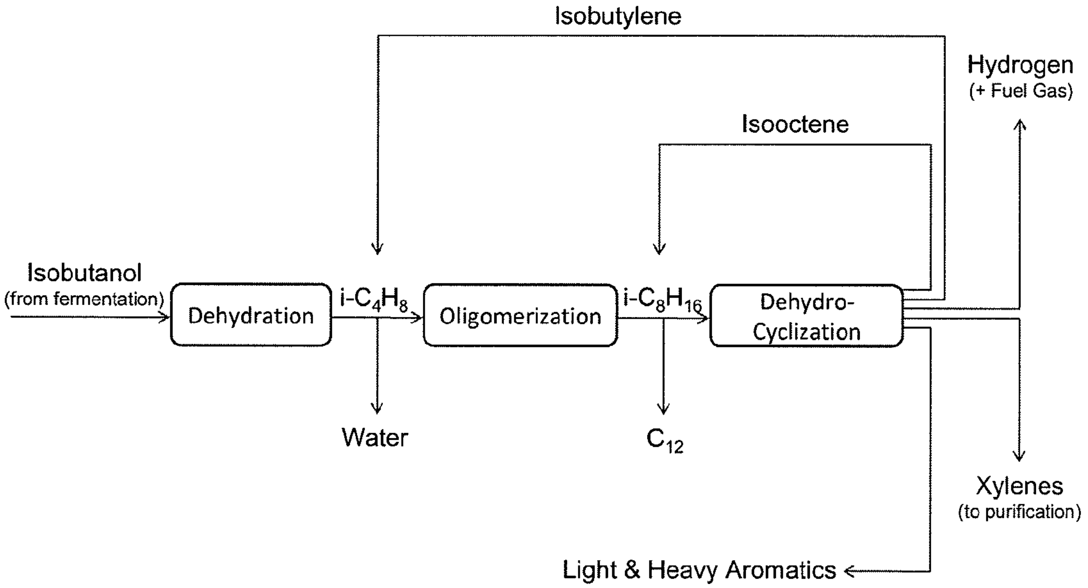


Figure 1: Process for Preparing p-Xylene from Isobutanol

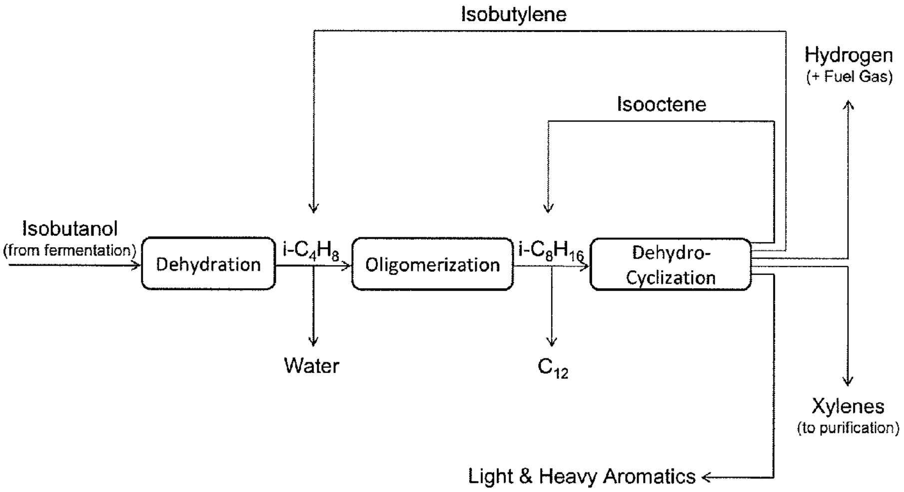


Figure 2: Single Pass Process for Preparing p-Xylene from Isobutanol

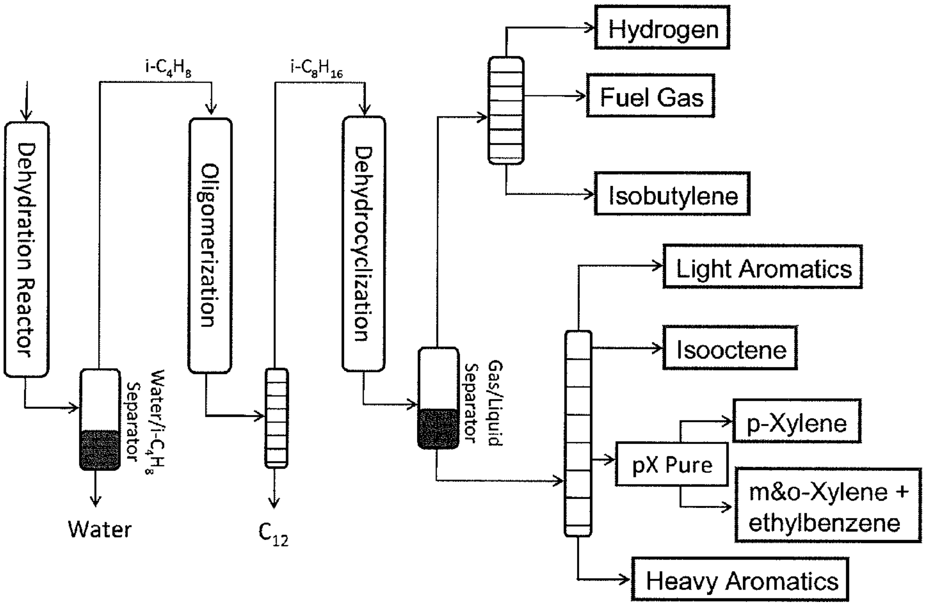
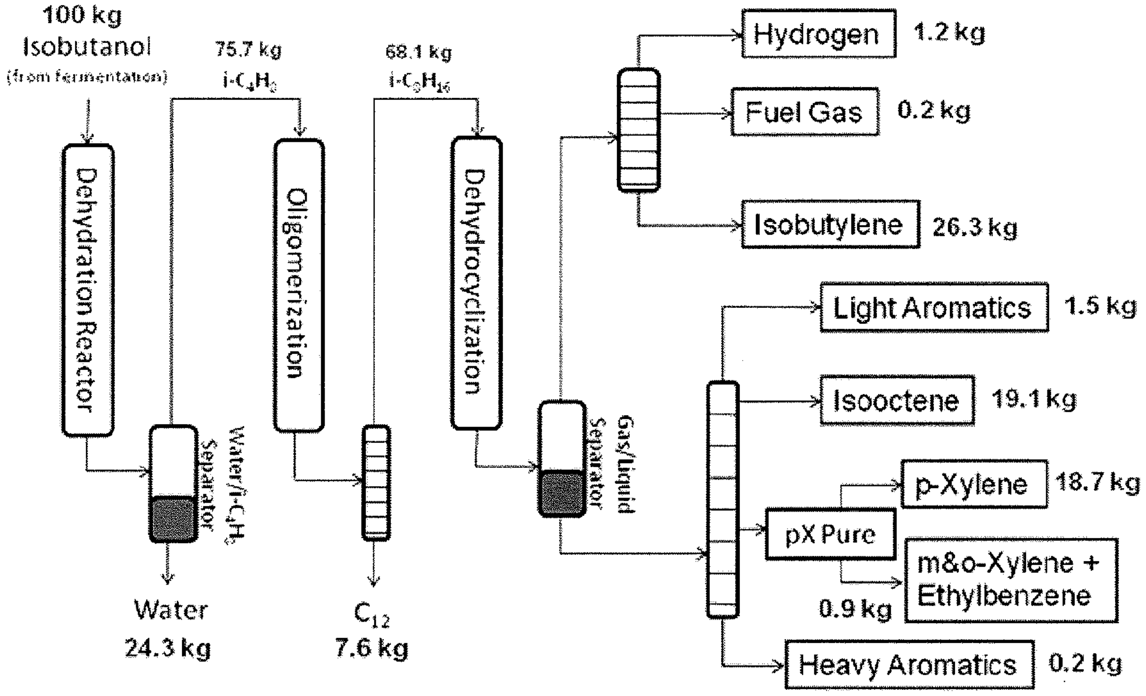


Figure 3: Single Pass Process for Preparing p-Xylene from Isobutanol (Including Yields)



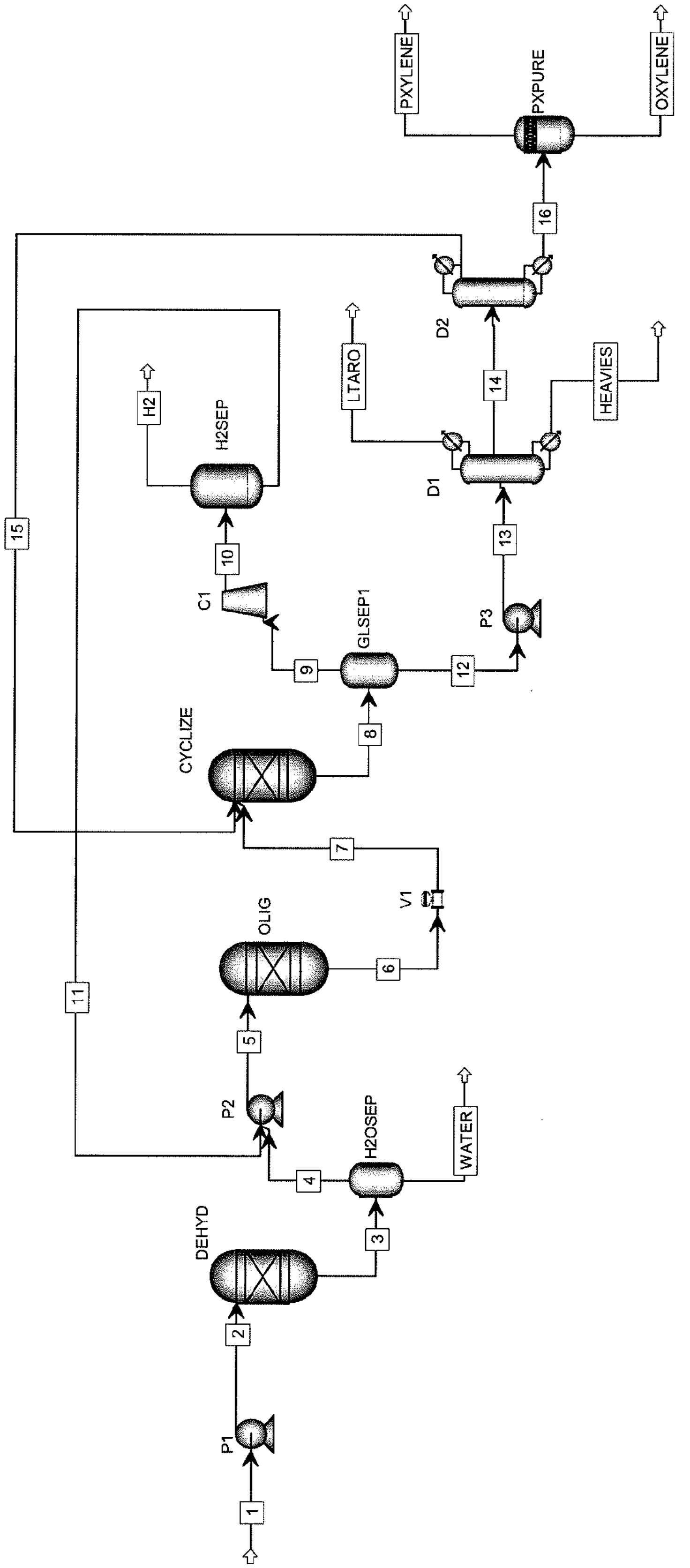


Figure 4: Integrated Process of Example 16

INTEGRATED PROCESS TO SELECTIVELY CONVERT RENEWABLE ISOBUTANOL TO P-XYLENE

CROSS REFERENCE TO RELATED APPLICATIONS

[0001] The present application claims priority to U.S. Provisional Application Nos. 61/249,078 filed Oct. 6, 2009, 61/295,886 filed Jan. 18, 2010, and 61/352,228 filed Jun. 7, 2010, the disclosures of each of which are herein incorporated by reference in their entireties for all purposes.

BACKGROUND OF THE INVENTION

[0002] Aromatic compounds are conventionally produced from petroleum feedstocks in refineries by reacting mixtures of light hydrocarbons (C_1-C_6) and naphthas over various catalysts at high heat and pressure. The mixture of light hydrocarbons available to a refinery is diverse, and provides a mixture of aromatic compounds (e.g., BTEX—benzene, toluene, ethylbenzene, and xylenes, as well as aromatic compounds having a molecular weight higher than xylenes). The xylenes product consists of three different aromatic C_8 isomers: p-xylene, o-xylene, and m-xylene; typically about one third of the xylenes are the p-xylene isomer. The BTEX mixture is then subjected to subsequent processes to obtain the desired product. For example, toluene can be removed and disproportionated to form benzene and xylene, or the individual xylene isomers can be isolated by fractionation (e.g. by absorptive separation, fractional crystallization, etc.). p-Xylene is the most commercially important xylene isomer, and is used almost exclusively in the production of polyester fibers, resins, and films. o-Xylene and m-xylene are also used in the production of phthalic anhydride, and isophthalic acid, respectively.

[0003] Alternatively, a single component feedstock purified from crude oil or synthetically prepared at the refinery can be selectively converted to purer aromatic product. For example, pure isooctene can be selectively aromatized to form primarily p-xylene over some catalysts (see, for example, U.S. Pat. No. 3,202,725, U.S. Pat. No. 4,229,320, U.S. Pat. No. 4,247,726, U.S. Pat. No. 6,600,081, and U.S. Pat. No. 7,067,708), and n-octane purified from crude oil can be converted to primarily o-xylene (see for example, U.S. Pat. No. 2,785,209).

[0004] Very high p-xylene purity is required to prepare terephthalic acid of suitable purity for use in polyester production—typically at least about 95% pure, or in some cases 99.7% or higher purity of p-xylene is required. Conventional processes for producing high purity p-xylene are thus complex and expensive: the conventional BTEX process requires isolation and extensive purification of p-xylene produced at relatively low levels; and alternative processes require isolation and purification of single component feedstocks for aromatization from complex hydrocarbon mixtures. Furthermore, production of p-xylene from conventional petroleum-based feedstocks contributes to environmental degradation (e.g., global warming, air and water pollution, etc.), and fosters over-dependence on unreliable petroleum supplies from politically unstable parts of the world. The present invention provides a simple process for preparing renewable, high purity p-xylene from renewable carbon sources, which can be converted to terephthalic acid and polyesters.

SUMMARY OF THE INVENTION

[0005] In one embodiment, the present invention is directed to a process for preparing renewable p-xylene comprising:

[0006] (a) treating biomass to form a fermentation feedstock;

[0007] (b) fermenting the fermentation feedstock with one or more species of microorganism to form a fermentation broth comprising aqueous isobutanol;

[0008] (c) removing aqueous isobutanol from the fermentation broth;

[0009] (d) dehydrating, in the presence of a dehydration catalyst, at least a portion of the aqueous isobutanol of step (c), thereby forming a dehydration product comprising one or more C_4 alkenes and water;

[0010] (e) dimerizing, in the presence of an oligomerization catalyst, a dimerization feedstock comprising at least a portion of the C_4 alkenes formed in step (d), thereby forming a dimerization product comprising one or more C_8 alkenes (optionally containing unreacted C_4 alkenes, and optionally comprising 2,4,4-trimethylpentenes, 2,5-dimethylhexene(s), and/or 2,5-dimethylhexadiene(s);

[0011] (f) dehydrocyclizing, in the presence of a dehydrocyclization catalyst, a dehydrocyclization feedstock comprising at least a portion of the C_8 alkenes of step (e), thereby forming a dehydrocyclization product comprising xylenes and hydrogen (and optionally one or more unreacted C_4 alkenes, unreacted 2,4,4-trimethylpentene(s), 2,5-dimethlyhexene(s), and/or 2,5-dimethylhexadiene(s)), wherein the xylenes comprise at least about 75% p-xylene.

[0012] In another embodiment, the present invention is also directed to methods for preparing renewable terephthalic acid from renewable p-xylene prepared by the method of the present invention.

[0013] In still another embodiment, the present invention is directed to methods for preparing renewable polyester terephthalate from the renewable terephthalic acid prepared by the method of the present invention.

BRIEF DESCRIPTION OF THE DRAWINGS

[0014] FIG. **1** is a schematic diagram of one embodiment of a process of the present invention for preparing p-xylene from isobutanol.

[0015] FIG. **2** is a schematic diagram of a single pass process according to the present invention for preparing p-xylene from isobutanol.

[0016] FIG. **3** is a schematic diagram of a single pass process according to the present invention for preparing p-xylene from isobutanol, which includes yields for various intermediates and products in the process.

[0017] FIG. **4** is a schematic diagram of an integrated process according to the present invention, as described in Example 15.

DETAILED DESCRIPTION OF THE INVENTION

[0018] All documents disclosed herein (including patents, journal references, ASTM methods, etc.) are each incorporated by reference in their entirety for all purposes.

[0019] The term "biocatalyst" means a living system or cell of any type that speeds up chemical reactions by lowering the activation energy of the reaction and is neither consumed nor altered in the process. Biocatalysts may include, but are not limited to, microorganisms such as yeasts, fungi, bacteria, and archaea.

[0020] The biocatalyst herein disclosed can convert various carbon sources into precursors for p-xylene. The term "carbon source" generally refers to a substance suitable for use as a source of carbon for prokaryotic or eukaryotic cell growth. Carbon sources include, but are not limited to biomass hydrolysates, starch, sucrose, cellulose, hemicellulose, xylose, and lignin, as well as monomeric components of these substrates (e.g., monosaccharides). Carbon sources can comprise various organic compounds in various forms including, but not limited to, polymers, carbohydrates, acids, alcohols, aldehydes, ketones, amino acids, peptides, etc. These include, for example, various monosaccharides such as glucose, dextrose (D-glucose), maltose, oligosaccharides, polysaccharides, saturated or unsaturated fatty acids, succinate, lactate, acetate, ethanol, etc., or mixtures thereof. Photosynthetic organisms can additionally produce a carbon source as a product of photosynthesis. In some embodiments, carbon sources may be selected from biomass hydrolysates and glucose.

[0021] The term "feedstock" is defined as a raw material or mixture of raw materials supplied to process for subsequent conversion into an intermediate or a final product. For example, a carbon source, such as biomass or the carbon compounds derived from biomass (e.g., a biomass hydrolysate as described herein) is a feedstock for a biocatalyst (e.g., a microorganism) in a fermentation process, and the resulting alcohol (e.g., isobutanol) produced by the fermentation can be a feedstock for subsequent unit operations (e.g., dehydration as described herein): e.g., isobutylene resulting from the dehydration of isobutanol can be a feedstock for dimerization, and the resulting diisobutylene (e.g., 2,4,4-trimethylpentene(s), 2,5-dimethylhexene(s), 2,5-dimethylhexadiene (s), etc.) can be a feedstock for dehydrocyclization. A feedstock may comprise one or more components. For example, the feedstock for a fermentation process (i.e., a fermentation feedstock) typically contains nutrients other than the carbon source; the feedstock for a dehydration unit operation typically also comprises water, the feedstock for dehydration typically also comprises water, the feedstock for dimerization typically also comprises diluents and unreacted isobutanol, and the feedstock for dehydrocyclization also typically comprises diluents, unreacted isobutanol and isobutylene, etc. The term "fermentation feedstock" is used interchangeably with the term "renewable feedstock", as fermentation feedstocks are generated from biomass or traditional carbohydrates, which are renewable substances.

[0022] The term "traditional carbohydrates" refers to sugars and starches generated from specialized plants, such as sugar cane, corn, and wheat. Frequently, these specialized plants concentrate sugars and starches in portions of the plant, such as grains, that are harvested and processed to extract the sugars and starches. Traditional carbohydrates such as those derived from corn are co-produced with food products derived from the protein-rich portion of the grains, and are primarily used as renewable feedstocks for fermentation processes to generate biofuels or fine chemicals (or precursors thereof).

[0023] Alternatively, renewable alcohols can be prepared photosynthetically, e.g., using cyanobacteria or algae engineered to produce isobutanol, isopentanol, and/or other alcohols (e.g., *Synechococcus elongatus* PCC7942 and *Synechocystis* PCC6803; see Angermayr et al., *Energy Biotechnology with Cyanobacteria*, Current Opinion in Biotechnology 2009, 20, 257-263, Atsumi and Liao, *Nature Biotechnology,* 2009, 27, 1177-1182); and Dexter et al., Energy Environ. Sci., 2009, 2, 857-864, and references cited in each of these references). When produced photosynthetically, the "feedstock" for producing the resulting renewable alcohols is light and the CO_2 provided to the photosynthetic organism (e.g., cyanobacteria or algae).

[0024] The term "biomass" as used herein refers primarily to the stems, leaves, and starch-containing portions of green plants, and is mainly comprised of starch, lignin, cellulose, hemicellulose, and/or pectin. Biomass can be decomposed by either chemical or enzymatic treatment to the monomeric sugars and phenols of which it is composed (Wyman, C. E. 2003 Biotechnological Progress 19:254-62). This resulting material, called biomass hydrolysate, is neutralized and treated to remove trace amounts of organic material that may adversely affect the biocatalyst, and is then used as a feedstock for fermentations using a biocatalyst. Alternatively, the biomass may be thermochemically treated to produce alcohols, alkanes, and alkenes that may be further treated to produce p-xylene.

[0025] The term "starch" as used herein refers to a polymer of glucose readily hydrolyzed by digestive enzymes. Starch is usually concentrated in specialized portions of plants, such as potatoes, corn kernels, rice grains, wheat grains, and sugar cane stems.

[0026] The term "lignin" as used herein refers to a polymer material, mainly composed of linked phenolic monomeric compounds, such as p-coumaryl alcohol, coniferyl alcohol, and sinapyl alcohol, which forms the basis of structural rigidity in plants and is frequently referred to as the woody portion of plants. Lignin is also considered to be the non-carbohydrate portion of the cell wall of plants.

[0027] The term "cellulose" as used herein refers is a long-chain polymer polysaccharide carbohydrate comprised of β-glucose monomer units, of formula $(C_6H_{10}O_5)_n$, usually found in plant cell walls in combination with lignin and any hemicellulose.

[0028] The term "hemicellulose" refers to a class of plant cell-wall polysaccharides that can be any of several heteropolymers. These include xylane, xyloglucan, arabinoxylan, arabinogalactan, glucuronoxylan, glucomannan and galactomannan. Monomeric components of hemicellulose include, but are not limited to: D-galactose, L-galactose, D-mannose, L-rhamnose, L-fucose, D-xylose, L-arabinose, and D-glucuronic acid. This class of polysaccharides is found in almost all cell walls along with cellulose. The molecular weight of hemicellulose is lower than for cellulose. Hemicellulose cannot be extracted with hot water or chelating agents, but can be extracted by aqueous alkali. Polymeric chains of hemicellulose bind pectin and cellulose in a network of cross-linked fibers forming the cell walls of most plant cells.

[0029] The term "pectin" as used herein refers to a class of plant cell-wall heterogeneous polysaccharides that can be extracted by treatment with acids and chelating agents. Typically, 70-80% of pectin is found as a linear chain of α-(1-4)-linked D-galacturonic acid monomers. The smaller RG-I fraction of pectin is comprised of alternating (1-4)-linked galacturonic acid and (1-2)-linked L-rhamnose, with substantial arabinogalactan branching emanating from the rhamnose residue. Other monosaccharides, such as D-fucose, D-xylose, apiose, aceric acid, Kdo, Dha, 2-O-methyl-D-fucose, and 2-O-methyl-D-xylose, are found either in the RG-II pectin fraction (<2%), or as minor constituents in the RG-I fraction. Proportions of each of the monosaccharides in relation to D-galacturonic acid vary depending on the individual plant and its micro-environment, the species, and time during the growth cycle. For the same reasons, the homogalacturonan and RG-I fractions can differ widely in their content of methyl esters on GalA residues, and the content of acetyl residue esters on the C-2 and C-3 positions of GalA and neutral sugars.

[0030] The term "yield" is defined as the amount of product obtained per unit weight of raw material and may be expressed as g product/g substrate. Yield may also be expressed as a percentage of the theoretical yield. "Theoretical yield" is defined as the maximum amount of product that can be generated per a given amount of substrate as dictated by the stoichiometry of the metabolic pathway used to make the product. For example, if the theoretical yield for one typical conversion of glucose to isobutanol is 0.41 g/g, the yield of isobutanol from glucose of 0.39 g/g would be expressed as 95% of theoretical or 95% theoretical yield.

[0031] The terms "alkene" and "olefin" are used interchangeably herein to refer to non-aromatic hydrocarbons having at least one carbon-carbon double bond.

[0032] "Renewably-based" or "renewable" denote that the carbon content of the indicated compound is from a "new carbon" source as measured by ASTM test method D 6866-08, "Standard Test Methods for Determining the Bio-Based Content of Solid, Liquid, and Gaseous Samples Using Radiocarbon Analysis". This test method measures the $^{14}C/^{12}C$ isotope ratio in a sample and compares it to the $^{14}C/^{12}C$ isotope ratio in a standard 100% biobased material to give percent biobased content of the sample. A small amount of the carbon atoms of the carbon dioxide in the atmosphere is the radioactive isotope ^{14}C. This ^{14}C carbon dioxide is created when atmospheric nitrogen is struck by a cosmic ray generated neutron, causing the nitrogen to lose a proton and form carbon of atomic mass 14 (^{14}C), which is then immediately oxidized to carbon dioxide. A small but measurable fraction of atmospheric carbon is present in the form of $^{14}CO_2$. Atmospheric carbon dioxide is processed by green plants to make organic molecules during the process known as photosynthesis. Virtually all forms of life on Earth depend on this green plant production of organic molecule to produce the chemical energy that facilitates growth and reproduction. Therefore, the ^{14}C that forms in the atmosphere eventually becomes part of all life forms and their biological products, enriching biomass and organisms which feed on biomass with ^{14}C. In contrast, carbon from "fossil" petroleum-based hydrocarbons does not have the signature ^{14}C:^{12}C ratio of renewable organic molecules derived from atmospheric carbon dioxide, because ^{14}C eventually decays to ^{14}N ($t_{1/2}$ of 5730 years).

[0033] "Biobased materials" are organic materials in which the carbon comes from recently (on a human time scale) fixated CO_2 present in the atmosphere using sunlight energy (photosynthesis). For example, a biobased hydrocarbon has a $^{14}C/^{12}C$ isotope ratio greater than 0. Contrarily, a fossil-based hydrocarbon has a $^{14}C/^{12}C$ isotope ratio of about 0. The term "renewable" with regard to compounds such as alcohols or hydrocarbons (e.g., alkenes, aromatics, etc.) refers to compounds prepared from biomass using thermochemical methods (e.g., gasification of biomass to form "syngas", which is subsequently reacted with Fischer-Tropsch catalysts to form e.g., hydrocarbons, alcohols, etc.), biocatalysts (e.g., fermentation), or other processes, for example as described herein.

[0034] The application of ASTM-D6866-08 to derive "biobased content" is built on the same concepts as radiocarbon dating, but without use of the age equations. The analysis is performed by deriving a ratio of the amount of radiocarbon (^{14}C) in an unknown sample compared to that of a modern reference standard. This ratio is reported as a percentage with the units "pMC" (percent modern carbon). If the material being analyzed is a mixture of present day radiocarbon and fossil carbon (containing very low levels of radiocarbon), then the pMC value obtained correlates directly to the amount of biomass material present in the sample.

[0035] The p-xylene prepared by the methods of the present invention has pMC values of at least about 1, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, inclusive of all values and subranges therebetween. In one embodiment, the pMC value of the p-xylene prepared by the methods of the present invention is greater than about 90; in another embodiment, the pMC value of the p-xylene prepared by the methods of the present invention is greater than about 95; in yet another embodiment, the pMC value of the p-xylene prepared by the methods of the present invention is greater than about 98; in still yet another embodiment, the pMC value of the p-xylene prepared by the methods of the present invention is greater than about 99; in a particular embodiment, the pMC value of the p-xylene prepared by the methods of the present invention is about 100.

[0036] The term "dehydration" refers to a chemical reaction that converts an alcohol into its corresponding alkene. For example, the dehydration of isobutanol produces isobutylene.

[0037] The term "dimerization" or "dimerizing" refer to oligomerization processes in which two identical activated molecules (such as isobutylene) are combined with the assistance of a catalyst (a dimerization catalyst or oligomerization catalyst, as described herein) to form a larger molecule having twice the molecular weight of either of the starting molecules (such as diisobutylene or 2,4,4-trimethylpentenes). The term "oligomerization" can be used to refer to a "dimerization" reaction, unless the formation of oligomers other than dimers is expressly or implicitly indicated.

[0038] The term "aromatization" refers to processes in which hydrocarbon starting materials, typically alkenes or alkanes are converted into one or more aromatic compounds (e.g., p-xylene) in the presence of a suitable catalyst by dehydrocyclization.

[0039] "Dehydrocyclization" refers to a reaction in which an alkane or alkene is converted into an aromatic hydrocarbon and hydrogen, usually in the presence of a suitable dehydrocyclization catalyst, for example any of those described herein.

[0040] The term "reaction zone" refers to the part of a reactor or series of reactors where the substrates and chemical intermediates contact a catalyst to ultimately form product. The reaction zone for a simple reaction may be a single vessel containing a single catalyst. For a reaction requiring two different catalysts, the reaction zone can be a single vessel containing a mixture of the two catalysts, a single vessel such as a tube reactor which contains the two catalysts in two separate layers, or two vessels with a separate catalyst in each which may be the same or different.

[0041] The phrase "substantially pure p-xylene" refers to isomeric composition of the xylenes produced by the dehydrocyclization step of the process. Xylenes which comprise "substantially pure p-xylene" comprise at least about 75% of the p-xylene isomer; and accordingly less than about 25% of the xylenes are other xylene isomers (e.g., o-xylene and m-xylene). Thus, xylenes comprising "substantially pure p-xylene" can comprise about 75%, about 80%, about 85%, about 90%, about 95%, about 96%, about 97%, about 98%, about 99%, about 99.5%, about 99.9%, or about 100% p-xylene.

[0042] The term "conversion" refers to the degree to which the reactants in a particular reaction (e.g., dehydration, dimerization, dehydrocyclization, etc.) are converted to products. Thus 100% conversion refers to complete consumption of reactants, and 0% conversion refers to no reaction.

[0043] The term "selectivity" refers to the degree to which a particular reaction forms a specific product, rather than another product. For example, for the dehydration of isobutanol, 50% selectivity for isobutylene means that 50% of the alkene products formed are isobutylene, and 100% selectivity for isobutylene means that 100% of the alkene products formed are isobutylene. Because the selectivity is based on the product formed, selectivity is independent of the conversion or yield of the particular reaction.

[0044] "WHSV" refers to weight hourly space velocity, and equals the mass flow (units of mass/hr) divided by catalyst mass. For example, in a dehydration reactor with a 100 g dehydration catalyst bed, an isobutanol flow rate of 500 g/hr would provide a WHSV of 5 hr^{-1}.

[0045] Unless otherwise indicated, all percentages herein are by weight (i.e., "wt. %).

[0046] In most embodiments, the fermentation feedstock comprises a carbon source obtained from treating biomass. Suitable carbon sources include any of those described herein such as starch, mono- and polysaccharides, pre-treated cellulose and hemicellulose, lignin, and pectin etc., which are obtained by subjecting biomass to one or more processes known in the art, including extraction, acid hydrolysis, enzymatic treatment, etc.

[0047] The carbon source is converted into a precursor of p-xylene (such as isobutanol) by the metabolic action of the biocatalyst (or by thermochemical methods, e.g. using gasification followed by chemical reaction over Fischer-Tropsch catalysts). The carbon source is consumed by the biocatalyst (e.g., a microorganism as described herein) and excreted as a p-xylene precursor (e.g., isobutanol) in a large fermentation vessel. The p-xylene precursor is then separated from the fermentation broth, optionally purified, and then subjected to further processes such as dehydration, dimerization, and aromatization to form aromatics comprising substantially pure p-xylene.

[0048] Depending on the biocatalyst, a particular C_4 alcohol or a mixture of C_4 alcohols can be obtained. For example, the biocatalyst can be a single microorganism capable of forming more than one type of C_4 alcohol during fermentation (e.g. two or more of 1-butanol, isobutanol, 2-butanol, t-butanol, etc.). In most embodiments however, it is most advantageous to obtain primarily one type of C_4 alcohol. In a particular embodiment, the C_4 alcohol is isobutanol. Accordingly, in most embodiments, a particular microorganism which preferentially forms isobutanol during fermentation is used.

[0049] Alternatively, renewable butanols (e.g., isobutanol) are prepared photosynthetically using an appropriate photosynthetic organism (cyanobacteria or algae as described herein).

[0050] Any suitable organism which produces a C_4 alcohol can be used in the fermentation step of the process of the present invention. For example, alcohols such as isobutanol are produced by yeasts during the fermentation of sugars into ethanol. Such alcohols (termed fusel alcohols in the art of industrial fermentations for the production of beer and wine) have been studied extensively for their effect on the taste and stability of these products. Recently, production of fusel alcohols using engineered microorganisms has been reported (U.S. Patent Publication No. 2007/0092957, and Nature, 2008, 451, p. 86-89). Isobutanol can be fermentatively produced by recombinant microorganisms as described in U.S. Provisional Patent Application No. 60/730,290 or in U.S. Patent Publ. Nos. 2009/0226990, 2009/0226991, 2009/0215137, 2009/0171129; 2-butanol can be fermentatively produced by recombinant microorganisms as described in U.S. Patent Application No. 60/796,816; and 1-butanol can be fermentatively produced by recombinant microorganisms as described in U.S. Provisional Patent Application No. 60/721,677. Other suitable microorganisms include those described, for example in U.S. Patent Publ. Nos. 2008/0293125, 2009/0155869.

[0051] The C_4 alcohol produced during fermentation can be removed from the fermentation broth by various methods, for example fractional distillation, solvent extraction (e.g., in particular embodiments with a renewable solvent such as renewable oligomerized hydrocarbons, renewable hydrogenated hydrocarbons, renewable aromatic hydrocarbons, etc. prepared as described herein), adsorption, pervaporation, etc. or by combinations of such methods, prior to dehydration. In other embodiments, the alcohol produced during fermentation is not isolated from the fermentation broth prior to dehydration, but is dehydrated directly as a dilute aqueous solution.

[0052] In a particular embodiment, the C_4 alcohol is removed by the process described in U.S. Patent Publ. No. 2009/0171129 A1. Specifically, the C_4 alcohol can be removed from the fermentation broth by either increasing the thermodynamic activity of the C_4 alcohol and/or decreasing the thermodynamic activity of the water, for example, maintaining the headspace of the fermentation vessel, or a side-stream of fermentation broth removed from the fermentation vessel (e.g., using a flash tank or other apparatus), at reduced pressure (e.g., below atmospheric pressure), and/or heating the side-stream of the fermentation broth, thereby providing a vapor phase comprising water and the C_4 alcohol (e.g., aqueous isobutanol). In a particular embodiment, the vapor phase provided thereby consists essentially of water and the C_4 alcohol. In yet another particular embodiment, the vapor phase provides an azeotropic mixture of the water and the C_4 alcohol. The vapor phase comprising the C_4 alcohol and water can be fed directly to the dehydration reaction step, or can be further concentrated by, for example cooling to condense the water and the C_4 alcohol to produce a two-phase liquid composition comprising a C_4 alcohol-rich phase, and a water-rich phase. The C_4 alcohol-rich liquid phase can then be separated from the water-rich phase using various methods known in the art, e.g., a liquid-liquid separator, etc. The aqueous C_4 alcohol removed from the fermentor can be further purified to remove water and/or other contaminants from the fermentation process, using conventional methods such as distillation, absorption, pervaporation, etc.

[0053] The removal of C_4 alcohol from the fermentation broth, as described herein, can occur continuously or semi-continuously. Removal of the C_4 alcohol in the manner described herein is advantageous because it provides for separation of the C_4 alcohol from the fermentation broth without the use of relatively energy intensive or equipment intensive unit operations such as distillation, pervaporation, absorption, etc., and removes a metabolic by-product of the fermentation, thereby improving the productivity of the fermentation process.

[0054] After removing the C_4 alcohol(s) from the fermentor, the C_4 alcohol(s) are converted to p-xylene by first catalytically dehydrating the alcohol to C_4 alkene(s) (isobutylene, 1-butene, and/or 2-butene), then catalytically dimerizing the C_4 alkene(s) to C_8 alkene(s) (linear or branched octenes, 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, 2,5-dimethylhexadienes, etc.). The C_8 alkene(s) are finally reacted in the presence of a dehydrocyclization catalyst to selectively form p-xylene. As is described in more detail herein, in particular embodiments the dehydration, dimerization, and dehydrocyclization reaction steps are carried out under reaction conditions which favor selectively forming specific products. For example, the dehydration reaction is carried out in the presence of a particular dehydration catalyst (as described herein), and under particular temperature, pressure, and WHSV conditions which selectively form isobutylene (e.g., at least about 95% of the C_4 alkenes formed are isobutylene); the dimerization reaction is carried out in the presence of a particular dimerization catalyst (as described herein), and under particular temperature, pressure, diluent and WHSV conditions which selectively form 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, and/or 2,5-dimethylhexadienes (e.g., at least about 50% of the C_8 alkenes formed are 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, and/or 2,5-dimethylhexadienes); and the dehydrocyclization reaction is carried out in the presence of a particular dimerization catalyst (as described herein), and under particular temperature, pressure, diluent and WHSV conditions which selectively form p-xylene (e.g., at least about 75% of the xylenes formed are p-xylene).

[0055] Selective dehydration, dimerization, and dehydrocyclization reaction steps are promoted by a variety of methods which reduce unwanted side-reactions (and the resulting undesirable by-products), such as the use of particularly selective catalysts, the addition of diluents, reduced reaction temperatures, reduced reactant residence time over the catalyst (i.e., higher WHSV values), etc. Such reaction conditions tend to reduce the percent conversion of particular reaction steps below 100%, and thus the feedstock for each successive reaction can include unreacted starting materials from the previous reaction step (which can function as diluents, as well as added diluents and by-products from previous reaction steps; For example, the feedstock for the dehydrocyclization reaction step can include the C_8 alkene produced by a dimerization reaction, as well as diluent gases (e.g., nitrogen, argon, and methane), unreacted C_4 alkene, etc. from the dimerization reaction, by-product C_4 and/or C_8 alkane from the dehydrocyclization reaction, etc. Unreacted starting materials can also be recycled back to the appropriate reaction step in order to boost the overall yield of p-xylene. For example, unreacted C_4 alkene present in the product stream from the dimerization reaction (or in some cases, also present in the product stream from the dehydrocyclization reaction) can be separated out of the product stream and recycled back to the feedstock for the dimerization reaction. In addition, C_4 and C_8 alkane by-products formed during the dehydrocyclization reaction (e.g., from the corresponding C_4 and C_8 alkenes present in the dehydrocyclization feedstock) can be recycled back to the feedstock for the dehydrocyclization reaction. C_8 alkanes (e.g., isooctane, 2,5-dimethylhexenes, 2,5-dimethylhexadienes, etc.) can react in the presence of the dehydrocyclization catalyst to form p-xylene, and C_4 alkene functions as a relatively inert diluent. The C_4 alkane can be recycled back to the feedstock of the oligomerization reaction where it acts as a diluent, which increases the selectivity of the oligomerization reaction, thereby providing products which are selectively dehydrocyclized to p-xylene.

[0056] The various reaction steps subsequent to production of the C_4 alcohol (e.g., dehydration, dimerization, and dehydrocyclization) can be carried out in a single reactor, within which the individual reaction steps take place in different reaction zones; or in which the catalysts are mixed or layered together in a single reaction zone, whereby the C_4 alcohol undergoes sequential conversion to successive intermediates in a single reaction zone (e.g., conversion of the C_4 alcohol to a C_4 alkene, then a C_8 alkene in a single reaction zone; or conversion of a C_4 alkene to a C_8 alkene, then dehydrocyclization of the C_8 alkene to p-xylene in a single reaction zone). Alternatively, the various reactions can be carried out in separate reactors so that the reactor conditions (e.g., temperature, pressure, catalyst, feedstock composition, WHSV, etc.) can be optimized to maximize the selectivity of each reaction step. When the separate reaction steps are carried out in separate reactors, the intermediates formed in the various reaction steps can be isolated and/or purified before proceeding to the subsequent reaction step, or the reaction product from one reactor can be passed directly to the subsequent reactor without purification.

[0057] In other embodiments of the processes of the present invention, one or more of the particular reaction steps (e.g., dehydration, dimerization, dehydrocyclization) can each be carried out in two or more reactors (connected either in series or in parallel), so that during operation of the process, particular reactors can be bypassed (or taken "offline") to allow maintenance (e.g., catalyst regeneration) to be carried out on the bypassed reactor, while still permitting the process to continue in the remaining operational reactors. For example, the dehydrocyclization step could be carried out in two reactors connected in series (whereby the product of the dimerization step is the feedstock for the first dehydrocyclization reactor, and the product of the first dehydrocyclization reactor is the feedstock for the second dehydrocyclization reactor). The first dehydrocyclization reactor can be bypassed using the appropriate piping and valves such that the product of the dehydrocyclization step is now the feedstock for the second dehydrocyclization reactor. For reactors connected in parallel, bypassing one of the reactors may simply entail closing the feed and product lines of the desired reactor. Such reactor configurations, and means for by-passing or isolating one or more reactors connected in series or parallel are known in the art.

[0058] The C_4 alcohol feedstock for the dehydration reaction can comprise a single C_4 alcohol (e.g., isobutanol) or can comprise a mixture of C_4 alcohols. In most embodiments, the dehydration feedstock comprises a single C_4 alcohol (e.g., isobutanol).

[0059] The dehydration reaction catalytically converts the C_4 alcohol produced in the fermentation step (e.g. isobutanol) into the corresponding C_4 alkene (e.g., isobutylene). Depending upon the dehydration catalyst used, dehydration of the C_4 alcohol can also be accompanied by rearrangement of the resulting C_4 alkene to form one or more isomeric alkenes. If isomerization occurs, the isomerization can occur concurrently with the dehydration, or subsequently to the dehydration.

[0060] The dehydration of alcohols to alkenes can be catalyzed by many different catalysts. In general, acidic heterogeneous or homogeneous catalysts are used in a reactor maintained under conditions suitable for dehydrating the C_4 alcohol. Typically, the C_4 alcohol is activated by an acidic catalyst to facilitate the loss of water. The water is usually removed from the dehydration reactor with the product. The resulting C_4 alkene either exits the reactor (e.g., in the gas or liquid phase depending upon the reactor conditions) and is captured by a downstream purification process or is further converted in the reactor to other compounds as described herein. For example, t-butyl alcohol is dehydrated to isobutylene by reacting it in the gas phase at 300-400° C. over an acid treated aluminum oxide catalyst (U.S. Pat. No. 5,625,109) or in the liquid phase at 120-200° C. over a sulfonic acid cationic exchange resin catalyst (U.S. Pat. No. 4,602,119). The water generated by the dehydration reaction exits the reactor with unreacted C_4 alcohol and C_4 alkene product and is separated by distillation or phase separation. Because water is generated in large quantities in the dehydration step, the catalysts used are generally tolerant to water and a process for removing the water from substrate and product may be part of any process that contains a dehydration step. For this reason, it is possible to use wet (i.e., up to 99% water by weight) C_4 alcohol as a substrate for a dehydration reaction and remove this water with the water generated by the dehydration reaction. For example, dilute aqueous solutions of ethanol (up to 98% water by weight) can be dehydrated over a zeolite catalyst with all water removed from the ethylene product stream after the dehydration step occurs (U.S. Pat. Nos. 4,698,452 and 4,873,392). Additionally, neutral alumina and zeolites will dehydrate alcohols to alkenes. For example, neutral chromium treated alumina will dehydrate isobutanol to isobutylene above 250° C. (U.S. Pat. No. 3,836,603).

[0061] Levels of water between about 0% and about 15% have little if any effect on the percent conversion and selectivity of the subsequent dehydration reaction. In most embodiments, the feedstock for the dehydration reaction comprises an aqueous C_4 alcohol comprising about 0-15% water, including about 0% water, about 1% water, about 2% water, about 3% water, about 4% water, about 5% water, about 6% water, about 7% water, about 8% water, about 9% water, about 10% water, about 11% water, about 12% water, about 13% water, about 14% water, or about 15% water, inclusive of all ranges and subranges therebetween. In a particular embodiment, the aqueous C_4 alcohol feedstock for the dehydration reaction comprises aqueous isobutanol containing about 0-15% water. In a specific embodiment, the dehydration reaction feedstock consists essentially of aqueous isobutanol containing about 0-15% water (e.g., about 85-100% isobutanol, and about 0-15% water), and trace levels of impurities (for example less than about 5% impurities, e.g., less than about 4%, less than about 3%, less than about 2%, or less than about 1% impurities).

[0062] Suitable dehydration catalysts include homogeneous or heterogeneous catalysts. A non-limiting list of homogeneous acid catalysts include inorganic acids such as sulfuric acid, hydrogen fluoride, fluorosulfonic acid, phosphotungstic acid, phosphomolybdic acid, phosphoric acid, Lewis acids such as aluminum and boron halides (e.g., $AlCl_3$, BF_3, etc.); organic sulfonic acids such as trifluoromethanesulfonic acid, p-toluenesulfonic acid and benzenesulfonic acid; heteropolyacids; fluoroalkyl sulfonic acids, metal sulfonates, metal trifluoroacetates, compounds thereof and combinations thereof. A non-limiting list of heterogeneous acid catalysts include heterogeneous heteropolyacids (HPAs); solid phosphoric acid; natural clay minerals, such as those containing alumina or silica; cation exchange resins such as sulfonated polystyrene ion exchange resins; metal oxides, such as hydrous zirconium oxide, Fe_2O_3, Mn_2O_3, γ-alumina, etc.; mixed metal oxides, such as sulfated zirconia/γ-alumina, alumina/magnesium oxide, etc.; metal salts such as metal sulfides, metal sulfates, metal sulfonates, metal nitrates, metal phosphates, metal phosphonates, metal molybdates, metal tungstates, metal borates; zeolites, such as NaY zeolite, H-ZSM-5, NaA zeolite, etc.; modified versions of any of the above known in the art, and combinations of any of the above, for example as described in U.S. Publ. Nos. 2009/0030239, 2008/0132741, 2008/0132732, 2008/0132730, 2008/0045754, 2008/0015395.

[0063] The dehydration reaction of the processes of the present invention is typically carried out using one or more fixed-bed reactors using any of the dehydration catalysts described herein. Alternatively, other types of reactors known in the art can be used, such as fluidized bed reactors, batch reactors, catalytic distillation reactors, etc. In a particular embodiment, the dehydration catalyst is a heterogeneous acidic γ-alumina catalyst. In order to maximize the purity of p-xylene ultimately produced, and to reduce or eliminate the need for purification of intermediates, it is desirable to carry out the dehydration reaction under conditions which favor selective formation of isobutylene. Higher selectivity is favored at lower conversion and under milder dehydration conditions (e.g., lower temperature and pressure).

[0064] In some embodiments, the dehydration reaction is carried out in the vapor phase to facilitate removal of water (either present in the dehydration feedstock or as a by-product of the dehydration reaction). In most embodiments, the dehydration reaction is carried out at a pressure ranging from 0-30 psig, and at a temperature of about 350° C. or less (e.g., about 300-350° C.). In other embodiments, the dehydration reaction pressure is about 0, about 5, about 10, about 15, about 20, about 25, or about 30, inclusive of all ranges and subranges therebetween. In most embodiments, the dehydration reaction temperature is about 325° C. or less, about 300° C. or less, about 275° C. or less, or about 250° C. or less. In a specific embodiment, the dehydration temperature is about 300° C. In another particular embodiment, the dehydration temperature is about 275° C. In still other embodiments, the dehydration temperature is at least about 100° C. and a pressure of at least about 1 atm.

[0065] The weight hourly space velocity (WHSV) of the dehydration reaction can range from about 1 to about 10 hr^{-1}, or about 1, about 2, about 3, about 4, about 5, about 6, about 7, about 8, about 9, or about 10 hr^{-1}. In a specific embodiment, the WHSV is about 5 hr^{-1}.

[0066] In still other embodiments, the dehydration reaction is carried out at higher pressures, ranging from about 60 psig to about 200 psig, for example at about 60 psig, about 70 psig, about 80 psig, about 90 psig, about 100 psig, about 110 psig, about 120 psig, about 130 psig, about 140 psig, about 150 psig, about 160 psig, about 170 psig, about 180 psig, about 190 psig, or about 200 psig, inclusive of all ranges and sub-ranges therebetween. When the dehydration reaction is carried out at such pressures, the isobutylene and water of the dehydration reaction product are separated in a liquid-liquid separator.

[0067] If the dehydration reaction product, or portions of the dehydration reaction product are produced in the vapor phase, the C_4 alkene (e.g. isobutylene) and water components of the dehydration reaction product can be separated by gas-liquid or liquid-liquid separation methods (i.e. after condensing the dehydration reaction product by cooling and/or compression). If the dehydration reaction product is substantially liquid, the product forms a C_4 alkene (e.g. isobutylene) rich phase and a water rich phase, which can be separated using a liquid-liquid separator.

[0068] In order for the processes of the present invention to ultimately provide substantially pure p-xylene, it is desirable to carry out the dehydration reaction under "selective" process conditions (e.g., choice of catalyst(s), temperature, pressure, WHSV, etc.) which provide a C_4 alkene product which is primarily isobutylene. In particular embodiments, the combination of temperature, pressure, catalyst used, and WHSV are selected such that the C_4 alkene product comprises at least about 95% isobutylene, e.g., temperatures of about 300° C. or lower, pressures of about 0-80 psig, catalysts such as BASF AL-3996, and a WHSV of about 5 hr^{-1}. In other particular embodiments, the C_4 alkene product comprises at least about 96%, at least about 97%, at least about 98%, at least about 99%, or about 100% isobutylene, inclusive of all ranges and sub-ranges therebetween.

[0069] The water produced in the dehydration reaction can be separated from the C_4 alkene (e.g., isobutylene) by various methods. For example, if the dehydration reaction is carried out at pressures of about 0-30 psig, the C_4 alkene can be separated as a gas from liquid water using a gas-liquid separator. When the dehydration reaction is carried out at pressures of about 30-100 psig, both the C_4 alkene and water can be condensed (e.g., by cooling or compressing the product stream) and the separation carried out using a liquid-liquid separator. In particular embodiments, the C_4 alkene (e.g., isobutylene) and water are separated after dehydration by gas-liquid separation. In some embodiments, unreacted C_4 alcohol is recycled back to the dehydration feedstock after separation from the C_4 alkene.

[0070] In particular embodiments, the dehydration reaction is run at temperature/pressure conditions (e.g., temperatures of about 250-350° C., pressures of 60-200 psig, WHSV of about 1-20 hr^{-1}). The C_4 alkene (e.g., isobutylene) product is then separated from the aqueous phase using a liquid-liquid separator. At least a portion of the unreacted isobutanol can be recycled back to the dehydration reaction feed; a portion of the unreacted isobutanol remaining in the C_4 alkene product mixture can also be retained in the dehydration product stream, and act as a diluent and/or modifier in the dimerization feedstock to improve selectivity of the dimerization reaction step.

[0071] In another particular embodiment, the dehydration reaction is carried out in multiple separate reactors (e.g., two, three, or more dehydration reactors) connected in series, wherein the temperature of the reactors increases in each successive dehydration reactor. When configured in this manner, one or more of the dehydration reactors can be bypassed during operation to permit e.g., regeneration of a "coked" catalyst in the bypassed reactor, without requiring a shutdown of the overall process.

[0072] In other embodiments, instead of recycling the unreacted isobutanol from the dehydration product stream, at least a portion of the unreacted isobutanol obtained after separation from the C_4 alkene (e.g., by liquid-liquid or gas-liquid separation) can be further dehydrated in additional dehydration reactors, and the resulting C_4 alkene product added to the feedstock for the dimerization step.

[0073] In most embodiments the dehydration and dimerization steps are carried out separately. In other embodiments, the dehydration and dimerization reactions are carried out in a single reaction zone using a catalyst (or mixture of catalysts) which catalyzes both reactions. The C_4 alkene(s) formed in the dehydration step can be transferred directly to the oligomerization catalyst (e.g., in another reaction zone or another reactor), or can be isolated prior to dimerization. In one embodiment, the C_4 alkene is isolated as a liquid and optionally purified (e.g., by distillation) prior to dimerization. Isolation of the C_4 alkene can be advantageous if the dehydration process is optimally carried out under gas-phase conditions, whereas the dimerization is optimally carried out under liquid-phase conditions; thus isolation of the C_4 alkene allows the dehydration and dimerization reactions to each be carried out under optimal conditions. Isolation of the C_4 alkene can refer to a process in which the C_4 alcohol produced by the biocatalyst (or thermochemical process) is continuously removed from the fermentor (as described herein) and dehydrated continuously to provide C_4 alkene. The C_4 alkene can then be stored and later reacted further (e.g., oligomerization and/or aromatization and/or hydrogenation and/or oxidation), or the isolated C_4 alkene can be temporarily stored in a holding tank prior to e.g. oligomerization providing an integrated, continuous process in which each of the unit operations (e.g., fermentation, dehydration, oligomerization, dehydrocyclization, etc.) run simultaneously and more or less continuously, and the isolation of the C_4 alkene "buffers" process upsets.

[0074] The oligomerization catalyst catalyzes dimerization, trimerization, etc. of the C_4 alkene. In the process of the present invention, primarily dimerization of the C_4 alkene to C_8 alkene(s) (e.g., 2,4,4-trimethylpentenes, etc.) is favored by appropriate selection of oligomerization catalyst and process conditions. In most embodiments, the dimerization reaction step is carried out under conditions which favor substantially exclusive dimer product (i.e., at least about 90% of the oligomers formed are C_8 alkene, at least about 95% of the oligomers formed are C_8 alkene, at least about 98% of the oligomers formed are C_8 alkene, at least about 99% of the oligomers are C_8 alkene, or about 100% of the oligomers formed are C_8 alkene). The unreacted C_4 alkene is then recycled.

[0075] Furthermore, the dimerization process is carried under selective conditions in which the C_8 alkene formed comprises primarily 2,4,4-trimethylpentenes; that is, the C_8 alkene dimers comprise at least about 50% 2,4,4-trimethylpentenes, or at least about 55%, at least about 60%, at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, at least about 90%, at least about 95%, or about 100% 2,4,4-trimethylpentenes.

[0076] In other embodiments, the dimerization process is carried under selective conditions in which the C_8 alkene formed comprises primarily 2,5-dimethylhexenes; that is, the C_8 alkene dimers comprise at least about 50% 2,5-dimethylhexenes, or at least about 55%, at least about 60%, at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, at least about 90%, at least about 95%, or about 100% 2,5-dimethylhexenes.

[0077] In still other embodiments, the dimerization process is carried under selective conditions in which the C_8 alkene formed comprises primarily 2,5-dimethylhexadienes; that is, the C_8 alkene dimers comprise at least about 50% 2,5-dimethylhexadienes, or at least about 55%, at least about 60%, at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, at least about 90%, at least about 95%, or about 100% 2,5-dimethylhexadienes.

[0078] In further embodiments, the dimerization process is carried under selective conditions in which the C_8 alkene formed comprises primarily 2,5-dimethylhexenes and 2,5-dimethylhexadienes; that is, the C_8 alkene dimers comprise at least about 50% 2,5-dimethylhexenes and 2,5-dimethylhexadienes, or at least about 55%, at least about 60%, at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, at least about 90%, at least about 95%, or about 100% 2,5-dimethylhexenes and 2,5-dimethylhexadienes.

[0079] At the high conversion conditions typical in petrochemical processing (e.g., >95% conversion), the oligomerization product typically comprises a mixture of isooctenes and isododecenes, which would require isolation and purification of the isooctene component prior to dehydrocyclization in order to provide sufficiently pure p-xylene. The selective dimerization conditions as described herein provide high levels of diisobutylene, for example 2,4,4,-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes, which can be converted subsequently to substantially pure p-xylene by dehydrocyclization as described herein. Selective dimerization conditions which produce essentially exclusively dimer alkene product, comprising at least about 50% 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes (or in other embodiments, at least about 55%, at least about 60%, at least about 65%, at least about 70%, at least about 75%, at least about 80%, at least about 85%, at least about 95%, at least about 95%, or about 100% 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes, inclusive of all ranges and subranges therebetween) are provided by various means, for example catalyst selection, choice of temperature and/or pressure, WHSV, the presence of diluents and modifiers, and combinations thereof. Suitable selective dimerization conditions include, for example dimerization with an Amberlyst strongly acidic ionic exchange resin catalyst at a temperature of about 100-120° C., approximately atmospheric pressure, WHSV of about 10-50 hr^{-1}, and a feedstock comprising about 50-90% diluents; for a ZSM-5 catalyst (e.g. CBV 2314), suitable dimerization conditions include a reaction temperature of about 150-180° C., a pressure of about 750 psig, a WHSV of about 10-100 hr^{-1}, and a feedstock comprising about 30-90% diluents; and for a solid phosphoric acid catalyst, suitable conditions include a reaction temperature of about 160-190° C., a pressure of about 500-1000 psig, WHSV of about 10-100 hr^{-1}, and a feedstock comprising about 25-75% diluents.

[0080] A non-limiting list of suitable acidic oligomerization catalysts includes inorganic acids, organic sulfonic acids, heteropolyacids, perfluoroalkyl sulfonic acids, metal salts thereof, mixtures of metal salts, and combinations thereof. The acid catalyst may also be selected from the group consisting of zeolites such as CBV-3020, ZSM-5, β Zeolite CP 814C, ZSM-5 CBV 8014, ZSM-5 CBV 5524 G, and YCBV 870; fluorinated alumina; acid-treated silica; acid-treated silica-alumina; acid-treated titania; acid-treated zirconia; heteropolyacids supported on zirconia, titania, alumina, silica; and combinations thereof. The acid catalyst may also be selected from the group consisting of metal sulfonates, metal sulfates, metal trifluoroacetates, metal triflates, and mixtures thereof; mixtures of salts with their conjugate acids, zinc tetrafluoroborate, and combinations thereof.

[0081] Other acid catalysts that may be employed in dimerization step of the invention include inorganic acids such as sulfuric acid, phosphoric acid (e.g., solid phosphoric acid), hydrochloric acid, and nitric acid, as well as mixtures thereof. Organic acids such as p-toluene sulfonic acid, triflic acid, trifluoroacetic acid and methanesulfonic acid may also be used. Moreover, ion exchange resins in the acid form may also be employed. Hence, any type of suitable acid catalyst known in the art may be employed.

[0082] Fluorinated sulfonic acid polymers can also be used as acidic oligomerization catalysts for the dimerization step of the processes of the present invention. These acids are partially or totally fluorinated hydrocarbon polymers containing pendant sulfonic acid groups, which may be partially or totally converted to the salt form. One suitable fluorinated sulfonic acid polymer is Nafion® perfluorinated sulfonic acid polymer, (E.I. du Pont de Nemours and Company, Wilmington, Del.). Another suitable fluorinated sulfonic acid polymer is Nafion® Super Acid Catalyst, a bead-form strongly acidic resin which is a copolymer of tetrafluoroethylene and perfluoro-3,6-dioxa-4-methyl-7-octene sulfonyl fluoride, converted to either the proton (H+), or the metal salt form.

[0083] A soluble acidic oligomerization catalyst may also be used in the method of the invention. Suitable soluble acids include, those acid catalysts with a pKa less than about 4, preferably with a pKa less than about 2, including inorganic acids, organic sulfonic acids, heteropolyacids, perfluoroalkylsulfonic acids, and combinations thereof. Also suitable are metal salts of acids with pKa less than about 4, including metal sulfonates, metal sulfates, metal trifluoroacetates, metal triflates, and mixtures thereof, including mixtures of salts with their conjugate acids. Specific examples of suitable acids include sulfuric acid, fluorosulfonic acid, phosphoric acid, p-toluenesulfonic acid, benzenesulfonic acid, phosphotungstic acid, phosphomolybdic acid, trifluoromethanesulfonic acid, 1,1,2,2-tetrafluoroethanesulfonic acid, 1,1,1,2,3,3-hexafluoropropanesulfonic acid, bismuth triflate, yttrium triflate, ytterbium triflate, neodymium triflate, lanthanum triflate, scandium triflate, zirconium triflate, and zinc tetrafluoroborate.

[0084] For batch reactions, the acidic oligomerization catalyst is preferably used in an amount of from about 0.01% to about 50% by weight of the reactants (although the concentration of acid catalyst may exceed 50% for reactions run in continuous mode using a packed bed reactor). In a particular embodiment, the range is 0.25% to 5% by weight of the reactants unless the reaction is run in continuous mode using a packed bed reactor. For flow reactors, the acid catalyst will be present in amounts that provide WHSV values ranging from about 0.1 hr^{-1} to 500 hr^{-1} (e.g., about 0.1, about 0.5, about 1.0, about 2.0, about 5.0, about 10, about 20, about 30, about 40, about 50, about 60, about 70, about 80, about 90, about 100, about 150, about 200, about 250, about 300, about 350, about 400, about 450, or about 500 hr^{-1}).

[0085] Other suitable heterogeneous acid catalysts include, for example, acid treated clays, heterogeneous heteropolyacids and sulfated zirconia. The acid catalyst can also be selected from the group consisting of sulfuric acid-treated silica, sulfuric acid-treated silica-alumina, acid-treated titania, acid-treated zirconia, heteropolyacids supported on zirconia, heteropolyacids supported on titania, heteropolyacids supported on alumina, heteropolyacids supported on silica, and combinations thereof. Suitable heterogeneous acid catalysts include those having an H_0 of less than or equal to 2.

[0086] In most embodiments of the present invention, the dimerization reaction step is typically carried out using a fixed-bed reactor using any of the oligomerization catalysts described herein. Alternatively, other types of reactors known in the art can be used, such as fluidized bed reactors, batch reactors, catalytic distillation reactors, etc. In a particular embodiment, the oligomerization catalyst is acidic catalyst such as HZSM-5, solid phosphoric acid, or a sulfonic acid resin.

[0087] As described above, the feedstock for the dimerization reaction step is obtained from the product of the dehydration reaction step (e.g., obtained after separating the C_4 alkene product from any unreacted isobutanol). If the dehydration reaction is carried out at pressures below about 30 psig, the C_4 alkene product obtained after gas-liquid separation can be compressed to form a C_4 alkene-rich feedstock for the dimerization reaction. Alternatively, if the dehydration reaction is carried out at higher pressures (e.g., about 60 psig or higher) and/or the dehydration product is separated using liquid-liquid separation, the liquid C_4 alkene-rich phase can be used as the feedstock for the dimerization reaction directly (e.g., pumped directly into the dimerization reactor), or can be diluted with suitable diluents as described herein. In particular embodiments, the liquid C_4 alkene-rich feedstock contains unreacted isobutanol from the dehydration reaction, and/or additional diluents added to improve the selectivity of the dimerization reaction step. In most embodiments, the C_4 alkene comprises isobutylene. In typical embodiments, it is desirable that the C_4 alkene portion of the feedstock comprises at least about 95% isobutylene, or at least about 96%, at least about 97%, at least about 98%, at least about 99%, or about 100% isobutylene.

[0088] As discussed herein, higher selectivity for formation of dimers such as 2,4,4-trimethylpentenes, 2,5 dimethylhexenes, and 2,5-dimethylhexadienes is favored at lower conversion and under milder oligomerization conditions (e.g., lower temperature and pressure). In most embodiments, the reaction is carried out in the liquid phase at a pressure ranging from 0-1500 psig, and at a temperature of about 250° C. or less. In some embodiments, the oligomerization reaction pressure is about 0, about 15, about 30, about 45, about 60, about 75, about 90, about 105, about 120, about 135, about 150, about 165, about 180, about 195, about 210, about 225, about 240, about 255, about 270, about 285, about 300, about 350, about 400, about 450, about 500, about 550, about 600, about 650, about 700, about 750, about 800, about 850, about 900, about 950, about 1000, about 1100, about 1200, about 1300, about 1400, or about 1500 psig, inclusive of all ranges and subranges therebetween.

[0089] In other embodiments, the dimerization reaction temperature is about 250° C. or less, about 225° C. or less, about 200° C. or less, about 175° C. or less, about 150° C. or less, about 125° C. or less, about 100° C. or less, about 75° C. or less, or about 50° C. or less, inclusive of all ranges and subranges therebetween. In a specific embodiment, the oligomerization temperature is about 170° C.

[0090] The weight hourly space velocity (WHSV) of the oligomerization reaction can range from about 1 hr^{-1} to about 500 hr^{-1}, or about 1, about 2, about 3, about 4, about 5, about 6, about 7, about 8, about 9, about 10, about 15, about 20, about 25, about 30, about 35, about 40, about 45, about 50, 55, about 60, about 65, about 70, about 75, about 80, about 85, about 90, about 95, about 100, about 110, about 120, about 130, about 140, about 150, about 175, about 200, about 225, about 250, about 275, about 300, about 350, about 400, about 450, or about 500 hr^{-1}. In a specific embodiment, the WHSV is about 5 hr^{-1}.

[0091] The renewable C_8 alkenes prepared after the oligomerization step in the process of the present invention have three, two or at least one double bond. On average, the product of the oligomerizing step of the process of the present invention has less than about two double bonds per molecule, in particular embodiments, less than about 1.5 double bonds per molecule. In most embodiments, the C_8 alkenes have on average one double bond.

[0092] Selective dimerization of the C_4 alkene during the dimerization reaction step can also be provided by the addition of alcohols such as t-butanol and diluents such as paraffins (such as kerosene, isooctane, or isobutane) to the oligomerization feedstock. In other embodiments, the selectivity of the dimerization reaction can be enhanced by adding water and isobutanol, e.g., by adding aqueous isobutanol, or by incompletely drying the C_4 alkene (isobutylene) product obtained from the dehydration reaction step (which contains unreacted isobutanol).

[0093] Some rearrangement of the C_4 alkene feedstock or C_8 alkene product may also occur during dimerization, thereby introducing new or undesired branching patterns into the C_8 alkene products. In most embodiments, rearrangement of the C_4 alkene feedstock and/or C_8 alkene product is not desirable, particularly when the oligomerization feedstock is isobutylene, and/or the oligomerization product is a 2,4,4-trimethylpentene, 2,5-dimethylhexene, or 2,5-dimethylhexadiene. In such embodiments, the reaction conditions and catalyst are selected to minimize or eliminate rearrangement (e.g., temperatures below at least about 200° C., or below about 180° C., and in particular embodiments, about 170° C.). In other embodiments, where the C_4 alkene feedstock includes some amount of unbranched C_4 alkene (i.e., 1-butene or 2-butene), the dimerization reaction could be carried out under conditions which favor dimerization and rearrangement to branched dimers such as 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes or under conditions in which linear butenes do not dimerize (or dimerize at a substantially lower rate compared to isobutylene), thereby maximizing the selectivity of the dimerization for 2,4,4-trimethylpentenes. Alternatively, the linear butenes could be isomerized by recycling the linear butenes to a separate isomerization reactor, after which the isomerized product (e.g., isobutylene) is then added back to the dimerization feedstock. Linear butene isomers can also be collected for use as a feedstock for other processes (for example, oligomerization to predominantly unbranched higher molecular weight hydrocarbons suitable for use as e.g. diesel fuel).

[0094] Similarly, if the C_8 alkene dimerization product is unbranched or includes C_8 isomers which do not dehydrocyclize selectively to p-xylene, it may be desirable to promote rearrangement of the dimerization feedstock to isobutylene and/or the dimerization product to 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes. Rearrangement to more desirable branched isomers (e.g., 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes) can be promoted by dimerization at lower temperatures and/or at higher WHSV values, or the less desirable C_8 alkene isomers can be isomerized by recycling back to the dimerization reactor, or by recycling to a separate isomerization reactor, after which the isomerized product (e.g., 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, or 2,5-dimethylhexadienes) is then added to the dehydrocyclization feedstock.

[0095] As discussed above, p-xylene (and other aromatics) are currently produced by catalytic cracking and catalytic reforming of petroleum-derived feedstocks. In particular, the catalytic reforming process uses light hydrocarbon "cuts" like liquefied petroleum gas (C_3 and C_4) or light naphtha (especially C_5 and C_6), which are then converted to C_6-C_8 aromatics, typically by one of the three main petrochemical processes such as M-2 Forming (Mobil), Cyclar (UOP) and Aroforming (IFP-Salutec). These processes use new catalysts which were developed to produce petrochemical grade benzene, toluene, and xylene (BTX) from low molecular weight alkanes in a single step. The process can be described as "dehydrogenation and dehydrocyclooligomerization" over one catalyst and in single reaction zone (the use of C_3 hydrocarbons requires oligomerization rather than dimerization to prepare substituted aromatics).

[0096] A variety of alumina and silica based catalysts and reactor configurations have been used to prepare aromatics from low molecular weight hydrocarbons. For example, the Cyclar process developed by UOP and BP for converting liquefied petroleum gas into aromatic compounds uses a gallium-doped zeolite (*Appl. Catal. A,* 1992, 89, p. 1-30). Other reported catalysts include bismuth, lead, or antimony oxides (U.S. Pat. No. 3,644,550 and U.S. Pat. No. 3,830,866), chromium treated alumina (U.S. Pat. No. 3,836,603 and U.S. Pat. No. 6,600,081), rhenium treated alumina (U.S. Pat. No. 4,229,320) and platinum treated zeolites (WO 2005/065393 A2). A non-limiting list of such catalysts include mixtures of chromia-alumina and bismuth oxide (e.g., bismuth oxide prepared by the thermal decomposition of bismuth compounds such as bismuth nitrate, bismuth carbonate, bismuth hydroxide, bismuth acetate, etc. and e.g., chromia-alumina prepared by impregnating alumina particles with a chromium composition to provide particles containing about 5, about 10, about 15, about 20, about 25, about 30, about 35, about 40, about 45, or about 50 mol % chromia, optionally including a promoter such as potassium, sodium, or silicon, and optionally including a diluent such as silicon carbide, α-alumina, zirconium oxide, etc.); bismuth oxide, lead oxide or antimony oxide in combination with supported platinum, supported palladium, supported cobalt, or a metal oxide or mixtures thereof, such as chromia-alumina, cobalt molybdate, tin oxide or zinc oxide; supported chromium on a refractory inorganic oxide such as alumina or zirconia, promoted with metal such as iron, tin, tungsten, optionally in combination with a Group I or II metal such as Na, K, Rb, Cs, Mg, Ca, Sr, and Ba); rhenium in oxide or metallic form deposited on a neutral or weakly acidic support which has been additionally impregnated with an alkali metal hydroxide or stannate and subsequently reduced with hydrogen at elevated temperatures; and platinum deposited on aluminosilicate MFI zeolite. Any of these known catalysts can be used in the process of the present invention. In particular embodiments of the process of the present invention, the dehydrocyclization catalyst includes, for example, chromium-oxide treated alumina, platinum- and tin-containing zeolites and alumina, cobalt- and molybdenum-containing alumina, etc. In a specific embodiment, the dehydrocyclization catalyst is a commercial catalyst based on chromium oxide on an alumina support.

[0097] High selectivity for p-xylene in the dehydrocyclization reaction is favored by providing a dehydrocyclization feedstock which comprises primarily 2,4,4-trimethylpentenes, 2,5-dimethlyhexenes, and/or 2,5-dimethylhexadienes by appropriate selection of dehydrocyclization catalyst (as described herein), and by appropriate selection of dehydrocyclization process conditions (e.g., process temperature, pressure, WHSV, etc.). In most embodiments, the dehydrocyclization reaction is carried out below or slightly above atmospheric pressure, for example at pressures ranging from about 1 psia to about 20 psia, or about 1 psia, about 2 psia, about 3 psia, about 4 psia, about 5 psia, about 6 psia, about 7 psia, about 8 psia, about 9 psia, about 10 psia, about 11 psia, about 12 psia, about 13 psia, about 14 psia, about 15 psia, about 16 psia, about 17 psia, about 18 psia, about 19 psia, and about 20 psia, inclusive of all ranges and subranges therebetween. In most embodiments, the dehydrocyclization is carried out at temperatures ranging from about 400° C. to about 600° C., or about 400° C., about 425° C., about 450° C., about 475° C., about 500° C., about 525° C., about 550° C., about 575° C., and about 600° C., inclusive of all ranges and subranges therebetween. In most embodiments, the dehydrocyclization is carried out at WHSV values of about 1 hr^{-1}, for example about 0.51 hr^{-1}, about 1 hr^{-1}, about 1.5 hr^{-1}, or about 2 hr^{-1}, inclusive of all ranges and subranges therebetween. In most embodiments, the dehydrocyclization reaction is operated at conversions ranging from about 20-50%, and provides a p-xylene selectivity (i.e., the percentage of xylene products which is p-xylene) greater than about 75%. In other embodiments, the p-xylene selectivity is $\geqq$about 75%, $\geqq$about 80%, $\geqq$about 85%, $\geqq$about 90%, $\geqq$about 95%, $\geqq$about 96%, $\geqq$about 97%, $\geqq$about 98%, or $\geqq$about 99%.

[0098] In addition, both the conversion and selectivity of the dehydrocyclization reaction for p-xylene can be enhanced by adding diluents to the feedstock, such as hydrogen, nitrogen, argon, and methane. Unreacted C_4 alkene (e.g. isobutylene from the oligomerization reaction) can also be used as an effective diluent to improve the p-xylene selectivity of the dehydrocyclization reaction, and to help suppress cracking. Accordingly, in some embodiments, the selectivity of the dimerization reaction step is improved by carrying out the dimerization under low conversion conditions, as discussed above, such that the product from the dimerization reaction contains significant amounts of unreacted C_4 alkene (e.g., isobutylene), a portion of which can be recycled back to the dimerization reaction feedstock, and a portion of which is present in the dehydrocyclization reaction feedstock. Any C_4 alkene (or C_4 alkane) remaining in the product of the dehydrocyclization reaction can then be recycled back into the dimerization feedstock and/or the dehydrocyclization feedstock. In some embodiments, the dehydrocyclization feedstock comprises 1-100% 2,4,4-trimethylpentenes, 2,5-dimethlyhexenes, and/or 2,5-dimethylhexadienes, with the balance diluent. In particular embodiments, the dehydrocyclization feedstock comprises less than about 50% 2,4,4-trimethylpentenes, 2,5-dimethlyhexenes, and/or 2,5-dimethylhexadienes to reduce "coking" of the dehydrocyclization catalyst. For example, the dehydrocyclization feedstock comprises about 1%, about 2%, about 5%, about 10%, about 15% about 20%, about 25%, about 30%, about 35%, about 40%, about 45%, or about 50% 2,4,4-trimethylpentenes, 2,5-dimethlyhexenes, and/or 2,5-dimethylhexadienes, inclusive of all ranges and sub-ranges therebetween.

[0099] The conversion of alkenes and alkanes into aromatic compounds is a net oxidation reaction that releases hydrogen from the aliphatic hydrocarbons. If no oxygen is present, hydrogen gas is a co-product, and light alkanes such as methane and ethane are by-products. If oxygen is present, the hydrogen is converted into water. The dehydrocyclization reaction step of the present invention is typically carried out in the relative absence of oxygen (although trace levels of oxygen may be present due to leaks in the reactor system, and/or the feedstock for the dehydrocyclization reaction step may have trace contamination with oxygen). The hydrogen and light hydrocarbons produced as a by-product of the dehydrocyclization reaction are themselves valuable compounds that can be removed and used for other chemical processes (e.g., hydrogenation of alkene by-products, for example C_8 alkenes such as 2,4,4-trimethylpentenes) to produce alkanes suitable for use as renewable fuels or renewable fuel additives (e.g., isooctane), etc.) in analogy to the practice in traditional petrochemical refineries that produces aromatics, these light compounds are collected and used throughout the refinery. This hydrogen also reacts with isobutylene and diisobutylene to produce isobutane and isooctane which can be recycled to use as diluents for oligomerization (isobutane and isooctane) or feedstock for dehydrocyclization to form isobutylene by dehydrogenation of isobutane and p-xylene by dehydrocyclization of isooctane. The mixture of hydrogen and light hydrocarbons produced from the dehydrocyclization reaction can be used for hydrogenation without further purification, or the light hydrocarbons can be removed (either essentially completely or a portion thereof) to provide relatively pure or higher purity hydrogen prior to the hydrogenation reaction.

[0100] Hydrogenation is carried out in the presence of a suitable active metal hydrogenation catalyst. Acceptable solvents, catalysts, apparatus, and procedures for hydrogenation in general can be found in Augustine, Heterogeneous Catalysis for the Synthetic Chemist, Marcel Decker, New York, N.Y. (1996).

[0101] Many hydrogenation catalysts known in the art are effective, including (without limitation) those containing as the principal component iridium, palladium, rhodium, nickel, ruthenium, platinum, rhenium, compounds thereof, combinations thereof, and the supported versions thereof.

[0102] Typically, the high temperatures at which these dehydrocyclization reactions are carried out tend to coke up and deactivate the catalysts. To reuse the catalyst, the coke must be removed as frequently as every 15 minutes, usually by burning it off in the presence of air. Thus, even though the dehydrocyclization reaction itself is, in most embodiments of the present invention, carried out in the absence of oxygen, oxygen (and optionally hydrogen) can periodically be introduced to reactivate the catalyst. The presence of hydrogenating metals such as nickel, platinum, and palladium in the catalyst will catalyze the hydrogenation of the coke deposits and extend catalyst life. In order to accommodate reactivation of the catalyst in a continuous process, two or more dehydrocyclization reactors can be used so that at least one dehydrocyclization reactor is operational while other dehydrocyclization reactors are taken "off line" in order to reactivate the catalyst. When multiple dehydrocyclization reactors are used, they can be connected in parallel or in series.

[0103] As discussed above, the hydrocarbon feedstocks used to form aromatic compounds in conventional petroleum refineries are typically mixtures of hydrocarbons. As a result, the p-xylene produced by petroleum refineries is mixed with other xylene isomers and other aromatics (e.g., light aromatics such as benzene and toluene, as well as ethylbenzene, etc.), requiring further separation and purification steps in order to provide suitably pure p-xylene for subsequent conversion to terephthalic acid or terephthalate esters suitable for polyester production. In a large-scale refinery, producing pure streams of p-xylene can be expensive and difficult. In contrast, the process of the present invention can readily provide relatively pure, renewable p-xylene at a cost which is competitive with that of petroleum derived p-xylene from conventional refineries.

[0104] For example, a biomass derived C_4 alcohol (e.g. aqueous isobutanol from fermentation) is dehydrated in the vapor phase over an acidic dehydration catalyst (e.g., gamma alumina) to form a product containing unreacted C_4 alcohol and 99% isobutylene (based on the total amount of olefin product). Isobutylene is removed from the dehydration product stream in the vapor phase from a condensed water/C_4 alcohol phase using e.g., a gas/liquid separator. Unreacted C_4 alcohol is recycled back into the dehydration reaction feedstock. Condensed isobutylene is then oligomerized to form diisobutylene (e.g., $\geqq$about 95% 2,4,4-trimethylpentenes) at about 50% conversion in an oligomerization reactor containing a metal-doped zeolite catalyst (e.g., HZSM-5). A portion of the unreacted isobutylene is recycled back to the oligomerization feedstock, while a remaining portion of the isobutylene remains in the product stream to serve as a diluent in the subsequent dehydrocyclization reaction step. The resulting mixture of diisobutylene and isobutylene, and optionally additional diluent (e.g., hydrogen, nitrogen, argon, and methane) is then fed into a dehydrocyclization reactor and reacted in the presence of a dehydrocyclization catalyst to selectively form p-xylene (e.g., >95% of the xylenes is p-xylene). Hydrogen produced as a co-product of the dehydrocyclization can be recycled back to the dehydrocyclization feedstock as a diluent, or alternatively used as a reactant to produce other compounds (e.g., to hydrogenate alkenes or alkene by-products for use as fuels or fuel additives, e.g., hydrogenate C_8 olefins such as isooctene to make isooctane for transportation fuels). Light alkanes in the hydrogen can be separated out before the purified hydrogen is utilized, or the impure light alkane/hydrogen mixture can be used directly in hydrogenation reactions. Unreacted isobutylene can be recycled back to the oligomerization feedstock, and/or fed to the dehydrocyclization feedstock as a diluent.

[0105] The resulting high purity p-xylene can be condensed from the product stream of the dehydrocyclization reaction and converted to terephthalic acid (TPA) or terephthalate esters (TPA esters) without further purification. However, since the purity requirements for TPA or TPA esters used as monomers in preparing PET is quite high (e.g., typically >about 99.5% purity), it may be desirable to further purify the renewable p-xylene prepared by the process of the present invention, e.g. by known methods such as simulated moving bed chromatography, fractional crystallization or fractional distillation. Although such methods are used in conventional petrochemical process for preparing high purity p-xylene, the "crude" p-xylene produced from the conventional process contains substantial amounts of impurities and undesirable xylene isomers (~10-30% impurities) and typically requires multiple purification steps to obtain the required purity level. In contrast, the "crude" p-xylene prepared by the process of the present invention is substantially more pure than conventional petrochemically produced p-xylene, and requires only minimal purification, if at all, to obtain purities suitable for preparing TPA or TPA ester monomers for polyester production.

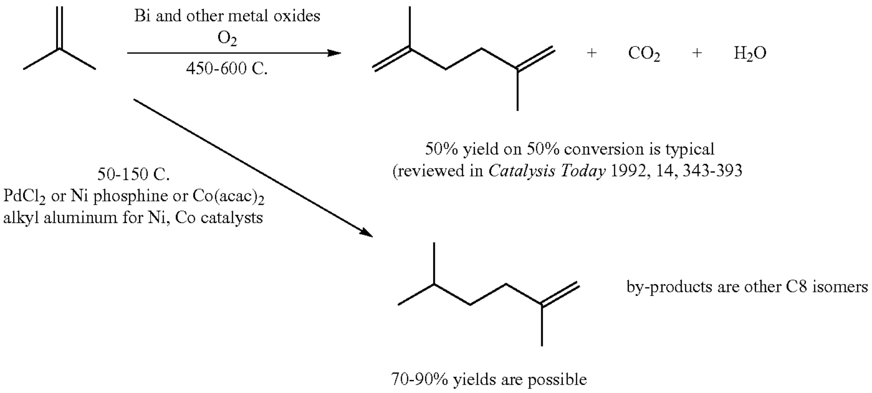
[0106] p-Xylene is converted into either TPA or TPA esters by oxidation over a transition metal-containing catalyst (*Ind. Eng. Chem. Res.* 2000, 39, p. 3958-3997 reviews the patent literature). Dimethyl terephthalate (DMT) has been traditionally produced at higher purity than TPA, and can be used to manufacture PET as well. Methods for producing TPA and DMT are taught in U.S. Pat. Nos. 2,813,119; 3,513,193; 3,887,612; 3,850,981; 4,096,340; 4,241,220; 4,329,493; 4,342,876; 4,642,369; and 4,908,471. TPA can be produced by oxidizing p-xylene in air or oxygen (or air or oxygen diluted with other gases) over a catalyst containing manganese and cobalt, although nickel catalysts have also been used with some success. Acetic acid is used as a solvent for these oxidation reactions and a bromide source such as hydrogen bromide, bromine, or tetrabromoethane is added to encourage oxidation of both methyl groups of the xylene molecule with a minimum of by-products. The temperatures of the reactions are generally kept between 80-270° C. with residence times of a few hours. The TPA is insoluble in acetic acid at lower temperatures (i.e. below 100° C.), which is how it is separated and purified. DMT can be produced by esterification of the "crude" product of the TPA reactions described above with methanol, and purification by distillation. A single step process to produce DMT by oxidizing p-xylene in the presence of methanol was developed by DuPont but is not often used due to low yields. All of these processes also produce monomethylesters of TPA which can be hydrolyzed to form the TPA or further esterified to form the diester, e.g., DMT.

[0107] Polyesters such as PET (polyethylene terephthalate) are prepared by polymerizing ethylene glycol with TPA or TPA esters, and thus 80% of the carbon content of PET resides in the terephthalate moiety of the polymer. Accordingly, PET prepared from renewable TPA or TPA esters, prepared as described herein, would comprise at least 80% renewable carbon. A completely renewable PET can be prepared by polymerizing TPA or TPA esters prepared according to the methods of the present invention with renewable ethylene glycol, prepared e.g. by the method of Mazloom et al., Iranian Polymer Journal, 16(9), 2007, 587-596; or Schonnagle et al., EP 1447506 A1.

[0108] Other renewable polymers, for example polyesters such as PTT (polytrimethylene terephthalate) or PBT (polybutylene terephthalate) can also be prepared from the renewable TPA or TPA esters as described herein by reaction of renewable TPA or TPA esters with any appropriate comonomer (e.g., 1,3-propylene glycol, butylene glycol, etc.) or other comonomers (polyols, polyamines, etc.) which react with TPA or TPA esters.

[0109] The processes of the present invention provide renewable p-xylene, which is environmentally advantageous compared to conventional processes for preparing p-xylene from petrochemical feedstock. In addition, the processes of the present invention are highly selective in forming p-xylene, whereas conventional petrochemical processes for preparing p-xylene are relatively nonselective overall. Conventional petrochemical processes for preparing high purity p-xylene are relatively nonselective and provide a mixture of aromatic compounds, from which the p-xylene must be isolated and purified to a level suitable for e.g., production of terephthalic acid. In addition, conventional petrochemical processes for preparing p-xylene often include unit operations for separating p-xylene from by-products such as benzene, toluene, ethylbenzene, and/or for converting such by-products to xylenes (including p-xylene), and/or for isomerizing o- and m-xylenes to p-xylene. In contrast, in various embodiments of the present invention can directly provide p-xylene of sufficient purity that such purification, conversion, and isomerization steps are generally not required. That is, in most embodiments, the processes of the present invention do not include steps of separating p-xylene from other xylene isomers, or separating p-xylene from other aromatic by-products (such as those described herein), or isomerizing by-product C_8 aromatics to p-xylene. In other embodiments, only minimal purification of the p-xylene is required (e.g., by separating the p-xylene from other xylene isomers or aromatic by-products).

[0110] The conversion of isooctene to p-xylene requires that typical multi-branched isooctene isomers such as 2,4,4-trimethylpentene are converted to 2,5-dimethylhexadiene before subsequent cyclization and dehydrogenation to p-xylene. When 2,5-dimethylhexadiene is reacted over the dehydrocyclization catalysts used to convert 2,4,4-trimethylpentenes to p-xylene, the 2,5-dimethylhexadiene is quantitatively converted into p-xylene whereas 2,4,4-trimethylpentene is at best only converted to p-xylene in 50% yield. To explain this fact, Anders, et al. (*Chemische Technik* 1986, 38, 116-119) propose a thermally catalyzed radical decomposition mechanism of 2,4,4-trimethylpentene which converts 2 equivalents of 2,4,4-trimethylpentene to 1 equivalent of 2,5-dimethylhexadiene and 2 equivalents of isobutane/isobutylene before conversion to p-xylene occurs under dehydrocyclization conditions. The isobutane/isobutylene produced from the reaction can be recycled to produce additional isooctene. To obtain high single pass yields from an isobutylene dimer, however, it is desired to first convert isobutylene directly to 2,5-dimethylhexadiene or 2,5-dimethylhexene then to pass the dimethylhexadiene or dimethylhexene over the dehydrocyclization catalyst to produce p-xylene in >50% yield. In the absence of oxygen, isobutylene is dimerized to 2,5-dimethylhexene over transition metal catalysts such as palladium(III) chloride or rhodium(III) chloride (e.g. French Patent 1499833A), cobalt(II) acetylacetonate and triethylaluminum (e.g. U.S. Pat. No. 5,320,993), or nickel with phosphorous and nitrogen chelating ligands (e.g. *Journal of Catalysis* 2004, 226, 235-239). Alternatively, dimerization/dehydrogenation of isobutylene to 2,5-dimethylhexadiene occurs in the presence of oxygen and a metal oxide catalyst, although at much lower yields than non-oxygenated processes. Multiple types of metal oxide and other metal catalysts including oxides, phosphides, and alloys of bismuth, tin, indium, thallium, antimony, cadmium, copper, iron, palladium, tungsten, niobium, arsenic, and niobium are used to dehydrodimerize olefins (e.g. *Catalysis Today* 1992, 14, 343-393). Both 2,5-dimethylhexadiene and 2,5-dimethylhexene are converted to p-xylene under the dehydrocyclization conditions described for 2,4,4-trimethylpentene with 2,5-dimethylhexene producing less hydrogen than the equivalent diene. In addition, the oxidative dehydrodimerization catalyst can be combined with a cyclizing catalyst (e.g., platinum on aluminum oxide, chromium on aluminum oxide, etc.) to increase the selectivity for cyclization to p-xylene. When the isobutylene converted to dimethylhexadiene or dimethylhexene is derived from renewable isobutanol, renewable p-xylene is obtained in high yield.



50% yield on 50% conversion is typical
(reviewed in *Catalysis Today* 1992, 14, 343-393

by-products are other C8 isomers

70-90% yields are possible

only Pd catalyst proven on isobutylene,
others are for ethylene dimerization
(e.g. FR1499833A, U.S. Pat. No. 5,320,993)

[0111] As discussed herein, the dimerization of C_4 alkenes to C_8 alkenes, and subsequent cyclodehydration to p-xylene can be carried out in a step-wise fashion, in which the dimerization product (comprising e.g., 2,4,4-trimethylpentenes, 2,5-dimethylhexenes, and/or 2,5-dimethylhexadienes) is isolated and optionally purified prior to cyclodehydration to p-xylene, or passed directly to the cyclodehydration reactor (or reaction zone) without isolation or purification. Alternatively, by appropriate selection of reaction conditions (i.e., catalyst(s), reaction temperature and pressure, reactor design, etc.) the dimerization and cyclodehydration reactions can be carried out essentially simultaneously, such that the C_4 alkene is effectively converted directly to p-xylene. In this regard, "essentially simultaneous" reaction steps could include direct conversion of the C_4 alkene (e.g., isobutylene) to p-xylene in a single reaction step, or rapid sequential conversion of the C_4 alkene to an intermediate (e.g., a C_8 alkene or other intermediate), which under the reaction conditions is rapidly converted to p-xylene such that no intermediates are isolated (or need be isolated).

[0112] For example, conversion of isobutylene directly to p-xylene can be carried out using a bismuth oxide catalyst under oxidative conditions, as described above, or alternatively reacting isobutylene, prepared as described herein, using conditions and catalysts used in petrochemical processes such as the M-2 Forming process (Mobil), Cyclar process (UOP) and Aroforming process (IFP-Salutec), to form an aromatic product comprising p-xylene.

EXAMPLES

Example 1

[0113] An overnight culture was started in a 250 mL Erlenmeyer flask with microorganism from a freezer stock (e.g., *Escherichia coli* modified to produce isobutanol, e.g., the organism described in U.S. Ser. No. 12/263,436) with a 40 mL volume of modified M9 medium consisting of 85 g/L glucose, 20 g/L yeast extract, 20 μM ferric citrate, 5.72 mg/L H_3BO_3, 3.62 mg/L $MnCl_2.4H_2O$, 0.444 mg/L $ZnSO_4.7H_2O$, 0.78 mg/L $Na_2MnO_4.2H_2O$, 0.158 mg/L $CuSO_4.5H_2O$, 0.0988 mg/L $CoCl_2.6H_2O$, 6.0 g/L $NaHPO_4$, 3.0 g/L KH_2PO_4, 0.5 g/L NaCl, 2.0 g/L NH_4Cl, 0.0444 g/L $MgSO_4$, and 0.00481 g/L $CaCl_2$ and at a culture OD_{600} of 0.02 to 0.05. The starter culture was grown for approximately 14 hrs in a 30° C. shaker at 250 rpm. Some of the starter culture was then transferred to a 400 mL DasGip fermentor vessel containing about 200 mL of modified M9 medium to achieve an initial culture OD_{600} of about 0.1. The vessel was attached to a computer control system to monitor and control the fermentation to a pH of 6.5 (by appropriate addition of base), a temperature of 30° C., dissolved oxygen levels, and agitation. The vessel was agitated, with a minimum agitation of 200 rpm—the agitation was varied to maintain a dissolved oxygen content of about 50% of saturation using a 12 sl/h air sparge until the OD_{600} was about 1.0. The vessel was then induced with 0.1 mM IPTG. After continuing growth for approximately 8-10 hrs, the dissolved oxygen content was decreased to 5% of saturation with 200 rpm minimum agitation and 2.5 sl/h airflow. Continuous measurement of the fermentor vessel off-gas by GC-MS analysis was performed for oxygen, isobutanol, ethanol, carbon dioxide, and nitrogen throughout the experiment. Samples were aseptically removed from the fermentor vessel throughout the fermentation and used to measure OD_{600}, glucose concentration, and isobutanol concentration in the broth. Isobutanol production reached a maximum at around 21.5 hrs with a titer of 18 g/L and a yield of approximately 70% maximum theoretical. The broth was subjected to vacuum distillation to provide a 84:16 isobutanol/water mixture which was redistilled as needed to provide dry isobutanol.

Example 2

[0114] GEVO1780 is a modified bacterial biocatalyst (described in U.S. Publ. No. 2009/0226990) that contains genes on two plasmids which encode a pathway of enzymes that convert pyruvate into isobutanol. When the biocatalyst GEVO1780 was contacted with glucose in a medium suitable for growth of the biocatalyst, at about 30° C., the biocatalyst produced isobutanol from the glucose. An overnight starter culture was started in a 250 mL Erlenmeyer flask with GEVO1780 cells from a freezer stock with a 40 mL volume of modified M9 medium consisting of 85 g/L glucose, 20 g/L yeast extract, 20 μM ferric citrate, 5.72 mg/L H_3BO_3, 3.62 mg/L $MnCl_2.4H_2O$, 0.444 mg/L $ZnSO_4.7H_2O$, 0.78 mg/L $Na_2MnO_4.2H_2O$, 0.158 mg/L $CuSO_4.5H_2O$, 0.0988 mg/L $CoCl_2.6H_2O$, $NaHPO_4$ 6.0 g/L, KH_2PO_4 3.0 g/L, NaCl 0.5 g/L, NH_4Cl 2.0 g/L, $MgSO_4$ 0.0444 g/L and $CaCl_2$ 0.00481 g/L and at a culture OD_{600} of 0.02 to 0.05. The starter culture was grown for approximately 14 hrs in a 30° C. shaker at 250 rpm. Some of the starter culture was then transferred to a 2000 mL DasGip fermenter vessel containing about 1500 mL of modified M9 medium to achieve an initial culture OD_{600} of about 0.1. The vessel was attached to a computer control system to monitor and control pH at 6.5 through addition of base, temperature at about 30° C., dissolved oxygen, and agitation. The vessel was agitated, with a minimum agitation of 400 rpm and agitation was varied to maintain a dissolved oxygen content of about 50% using a 25 sL/h air sparge until the OD_{600} was about 1.0. The vessel was then induced with 0.1 mM IPTG. After continuing growth for approximately 8-10 hrs, the dissolved oxygen content was decreased to 5% with 400 rpm minimum agitation and 10 sl/h airflow. Continuous measurement of the fermentor vessel off-gas by GC-MS analysis was performed for oxygen, isobutanol, ethanol, and carbon dioxide throughout the experiment. Samples were aseptically removed from the fermenter vessel throughout the experiment and used to measure OD_{600}, glucose concentration, and isobutanol concentration in the broth. Throughout the experiment, supplements of pre-grown and pre-induced biocatalyst cells were added as a concentrate two times after the start of the experiment: at 40 h and 75 h. These cells were the same strain and plasmids indicated above and used in the fermenter. Supplemented cells were grown as 1 L cultures in 2.8 L Fernbach flasks and incubated at 30° C., 250 RPM in Modified M9 Medium with 85 g/L glucose. Cultures were induced upon inoculation with 0.1 mM IPTG. When the cells had reached an OD_{600} of about 4.0-5.0, the culture was concentrated by centrifugation and then added to the fermenter. A glucose feed of about 500 g/L glucose in DI water was used intermittently during the production phase of the experiment at time points greater than 12 h to maintain glucose concentration in the fermenter of about 30 g/L or above.

[0115] The fermenter vessel was attached by tubing to a smaller 400 mL fermenter vessel that served as a flash tank and operated in a recirculation loop with the fermenter. The biocatalyst cells within the fermenter vessel were isolated from the flash tank by means of a cross-flow filter placed in-line with the fermenter/flash tank recirculation loop. The filter only allowed cell-free fermentation broth to flow from the fermenter vessel into the flash tank. The volume in the flash tank was approximately 100 mL and the hydraulic retention time was about 10 minutes. Heat and vacuum were applied to the flash tank. The vacuum level applied to the flash tank was initially set at about 50 mBar and the flash tank was set at about 45° C. These parameters were adjusted to maintain approximately 6-13 g/L isobutanol in the fermenter throughout the experiment. Generally, the vacuum ranged from 45-100 mBar and the flash tank temperature ranged from 43° C. to 45° C. throughout the experiment. Vapor from the heated flash tank was condensed into a collection vessel as distillate. Cell-free fermentation broth was continuously returned from the flash tank to the fermentation vessel.

[0116] The distillate recovered in the experiment was strongly enriched for isobutanol. Isobutanol formed an azeotrope with water and usually lead to a two phase distillate: an isobutanol rich top phase and an isobutanol lean bottom phase. Distillate samples were analyzed by GC for isobutanol concentration. Isobutanol production reached a maximum at around 118 hrs with a total titer of about 87 g/L. The isobutanol production rate was about 0.74 g/L/h on average over the course of the experiment. The percent theoretical yield of isobutanol was approximately 90.4% at the end of the experiment. The broth was subjected to vacuum distillation to provide a 84:16 isobutanol/water mixture which was redistilled as needed to provide dry isobutanol.

Example 3

Dry Isobutanol Dehydration

[0117] Dry isobutanol (<1 wt % water) obtained in Example 2 was fed through a preheater to a fixed-bed tubular reactor packed with a commercial γ-alumina dehydration catalyst (BASF AL-3996). The internal reactor temperature was maintained at 325° C. and the reactor pressure was atmospheric. The WHSV of the isobutanol was 5 hr^{-1}. Primarily isobutylene and water were produced in the reactor, and were separated in a gas-liquid separator at 20° C.; the water had <1% of unreacted isobutanol and the conversion was >99.8%. GC-FID analysis of the gas phase effluent indicated it was 95% isobutylene, 3.5% 2-butene (cis and trans) and 1.5% 1-butene.

Example 4

Wet Isobutanol Dehydration

[0118] Wet isobutanol (containing 15% water) obtained in Example 2 was fed through a preheater to a fixed-bed tubular reactor packed with a commercial dehydration catalyst (BASF AL-3996). The internal reactor temperature was maintained at 275° C. and the reactor pressure was atmospheric. The WHSV of the isobutanol was 10 hr^{-1}. Primarily isobutylene and water were produced in the reactor, and were separated in a gas-liquid separator at 20° C.; two liquid phases were recovered: one phase comprised water saturated with isobutanol and the other isobutanol-rich phase comprised isobutanol saturated with water. The isobutanol-rich phase was approximately 70% of the liquid effluent, indicating that isobutanol conversion in the reactor was approximately 40%. GC-FID analysis of the gas phase effluent indicated it was about 99% isobutylene, about 0.6% 2-butene (cis and trans) and about 0.4% 1-butene.

Example 5

Dry Isobutanol Dehydration at 60 psig

[0119] Dry isobutanol (<1 wt % water) obtained in Example 2 was fed through a preheater to a fixed-bed tubular reactor packed with a commercial γ-alumina dehydration catalyst (BASF AL-3996). The internal reactor temperature was maintained at 325° C. and the reactor pressure was maintained at 60 psig. The WHSV of the isobutanol was 5 hr^{-1}. Primarily isobutylene and water were produced in the reactor, and were separated in a liquid-liquid separator at 20° C.; the water had <1% of unreacted isobutanol and the conversion was >99.8%. GC-FID analysis of the gas phase effluent indicated it was 95% isobutylene, 3.5% 2-butene (cis and trans) and 1.5% 1-butene.

Example 6

Dry n-Butanol Dehydration at 60 psig

[0120] Dry n-butanol (<1 wt % water) is fed through a preheater to a fixed-bed tubular reactor packed with a commercial γ-alumina dehydration catalyst (BASF AL-3996). The internal reactor temperature is maintained at 450° C. and the reactor pressure is maintained at 60 psig. The WHSV of the isobutanol is 3 hr^{-1}. An equilibrium mixture of C_4 olefins and water are produced in the reactor, and are separated in a liquid-liquid separator at 20° C.; the water has <1% of unreacted isobutanol and the conversion is >99.8%. GC-FID analysis of the gas phase effluent indicates it is about 47% isobutylene, about 41% 2-butene (cis and trans) and about 12% 1-butene.

Example 7

Oligomerization of Isobutylene

[0121] The product stream from Example 3 was dried over molecular sieves, compressed to 60 psig, cooled to 20° C. so that the isobutylene was condensed to a liquid and pumped with a positive displacement pump into a fixed-bed oligomerization reactor packed with a commercial ZSM-5 catalyst (CBV 2314). The reactor was maintained at 175° C. and a pressure of 750 psig. The WHSV of the isobutylene-rich stream was 15 hr^{-1}. The reactor effluent stream was 10% unreacted butenes, 60% isooctenes (primarily 2,4,4-trimethylpentenes), 28% trimers, and 2% tetramers.

Example 8

Oligomerization of Isobutylene

[0122] The product stream from Example 5 (which was saturated with water) was pumped with a positive displacement pump into a fixed-bed oligomerization reactor packed with a commercial ZSM-5 catalyst (CBV 2314). The reactor was maintained at 170° C. and a pressure of 750 psig. The WHSV of the isobutylene-rich stream was 50 hr^{-1}. The reactor effluent stream was 20% unreacted butenes, 64% isooctenes (primarily 2,4,4-trimethylpentenes), 15% trimers, and 1% tetramers.

Example 9

Oligomerization of Isobutylene with Modifier

[0123] The product stream from Example 5 is co-fed with 2% wet isobutanol (by weight) and pumped with a positive displacement pump into a fixed-bed oligomerization reactor packed with a commercial ZSM-5 catalyst (CBV 2314). The reactor is maintained at 160° C. and a pressure of 750 psig. The WHSV of the isobutylene-rich stream is 200 hr^{-1}. The product stream is about 30% unreacted butenes, about 69% isooctenes (primarily 2,4,4-trimethylpentenes), and about 1% trimers.

Example 10

Oligomerization of Isobutylene with Diluents

[0124] The product stream from Example 3 is co-fed with 50% isobutane to a compressor, condensed and pumped into a fixed-bed oligomerization reactor packed with Amberlyst 35 (strongly acidic ionic exchange resin available from Rohm & Haas). The reactor is maintained at 120° C. and a pressure of 500 psig. The WHSV of the isobutylene-rich stream is 100 hr^{-1}. The product stream is about 50% isobutane (diluents), about 3% unreacted butenes, about 44% isooctenes (primarily 2,4,4-trimethylpentenes), and about 3% trimers.

Example 11

Oligomerization of Mixed Butenes

[0125] The product stream from Example 6 is pumped with a positive displacement pump into a fixed-bed oligomerization reactor packed with a commercial ZSM-5 catalyst (CBV 2314). The reactor is maintained at 170° C. and a pressure of 750 prig. The WHSV of the mixed butene stream is 20 hr^{-1}. The reactor effluent stream is about 60% unreacted butenes (primarily linear butenes), about 36% isooctenes (primarily 2,4,4-trimethylpentenes), and about 4% trimers.

Example 12

Recycle of Unreacted Linear Butenes

[0126] The product stream from Example 11 is distilled to recover the unreacted butenes (primarily linear butenes). The linear butene-rich stream is condensed and pumped with a positive displacement pump into an isomerization reactor at 450° C. where the equilibrium composition of mixed butenes is re-established. The mixed butene stream is recycled back and combined with the oligomerization reactor feed used in Example 10. The overall system conversion is >99% using the recycle stream and the yield of isooctenes is >89% with approximately 10% trimers.

Example 13

Dehydrocyclization of Isooctene

[0127] Isooctene from Example 7 was distilled to remove trimers and tetramers and then fed at a molar ratio of 1.3:1 mol nitrogen diluent gas to a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction was carried out at atmospheric pressure and a temperature of 550° C., with a WHSV of 1.1 hr^{-1}. The reactor product was condensed and analyzed by GC-MS. Of the xylene fraction, p-xylene was produced in greater than 80% selectivity. Analysis by method ASTM D6866-08 showed p-xylene to contain 96% biobased material.

Example 14

Dehydrocyclization of Isooctene with Diluents

[0128] The product from Example 10 containing 50% isobutane, 3% butenes, 44% isooctenes, and 3% trimers is fed to a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction is carried out at atmospheric pressure and a temperature of 525° C., with a WHSV of 1.1 hr^{-1}. The reactor product is condensed and analyzed by GC-MS. Of the xylene fraction, p-xylene is produced in greater than 85% selectivity. Hydrogen is also produced and captured for use with other processes.

Example 15

Dehydrocyclization of Isooctene with Diluents

[0129] Isooctene from Example 8 and diluent isobutylene from Example 5 are fed in a 1:1 molar ratio to a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction is carried out at atmospheric pressure and a temperature of 550° C., with a WHSV of 1.1 hr^{-1}. The reactor product is condensed and analyzed by GC-MS. Of the xylene fraction, p-xylene is produced in greater than 75% selectivity. Hydrogen is also produced and captured for use with other processes.

Example 16

Integrated System to Convert Isobutanol to Renewable p-Xylene

[0130] Renewable isobutanol is converted to renewable p-xylene using a process illustrated in FIG. **4**. Isobutanol (stream 1) from Example 1 or 2 is fed wet (15 wt % water) through a preheater into a fixed-bed catalyst reactor packed with a commercial γ-alumina catalyst (BASF AL-3996) at a WHSV of 10 hr^{-1}. The dehydration reactor is maintained at 290° C. at a pressure of 60 psig. The effluent (3) from the dehydration reactor is fed to a liquid/liquid separator, where water is removed. Analysis of the organic phase (4) shows that it is 95% isobutylene, 3% linear butenes, and 2% unreacted isobutanol. The organic phase is combined with a recycle stream (11) containing isobutane, isooctane, and unreacted butenes and fed to a positive displacement pump (P2) where it is pumped to an oligomerization reactor packed with HZSM-5 catalyst (CBV 2314) at a WHSV of 100 hr^{-1}. The reactor is maintained at 170° C. at a pressure of 750 psig. The effluent (6) from the oligomerization reactor is analyzed and shown to contain 60% unreacted feed (isobutane, isooctane, and butenes), 39% isooctene, and 1% trimers. The effluent from the oligomerization reactor is combined with recycled isooctene (15) and fed through a preheater and to a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛") at a WHSV of 1 hr^{-1}. The dehydrocyclization reactor is maintained at 550° C. and 5 psia. The yield of xylenes from the reactor relative to C_8 alkenes in the feed is 42% with a selectivity to p-xylene of 90%. The effluent (8) is separated with a gas-liquid separator. The gas-phase is compressed (C1) to 60 psig causing the isobutane and butenes to condense. A second gas-liquid separator is used to recover the hydrogen (and small quantities of methane or other light hydrocarbons). The C_4 liquids are recycled (11) and combined with the organic phase from the dehydration reactor (4). The liquid product (12) from the dehydrocyclization reactor is fed to a series of distillation columns slightly above atmospheric pressure by a pump (P3). Any by-product light aromatics (benzene and toluene) and heavy compounds (C_9+ aromatics or isoolefins) are removed. A side stream (14) rich in xylenes and iso-C_8 compounds are fed to a second distillation column. The C_8 compounds (isooctene and isooctane) are recycled (15) to the feed of the dehydrocyclization reactor. The xylene fraction (16) is fed to a purification process resulting in a 99.99% pure p-xylene product and a small byproduct stream rich in o-xylene.

Example 17

Oxidation of Renewable p-Xylene to Terephthalic Acid

[0131] A 300 mL Parr reactor was charged with glacial acetic acid, bromoacetic acid, cobalt acetate tetrahydrate, and p-xylene, obtained from Example 13, in a 1:0.01:0.025:0.03 mol ratio of glacial acetic acid:bromoacetic acid:cobalt acetate tetrahydrate:p-xylene. The reactor was equipped with a thermocouple, mechanical stirrer, oxygen inlet, condenser, pressure gauge, and pressure relief valve. The reactor was sealed and heated to 150° C. The contents were stirred and oxygen was bubbled through the solution. A pressure of 50-60 psi was maintained in the system and these reaction conditions were maintained for 4 h. After 4 h, the reactor was cooled to room temperature. Terephthalic acid was filtered from solution and washed with fresh glacial acetic acid.

Example 18

Purification of Renewable Terephthalic Acid

[0132] Terephthalic acid from Example 17 was charged to a 300 mL Parr reactor with 10% Pd on carbon catalyst in a 4.5:1 mol ratio of terephthalic acid: 10% Pd on carbon. Deionized water was charged to the reactor to make a slurry containing 13.5 wt. % terephthalic acid. The reactor was equipped with a thermocouple, mechanical stirrer, nitrogen inlet, hydrogen inlet, pressure gauge, and pressure relief valve. The Parr reactor was sealed and flushed with nitrogen. The Parr reactor was then filled with hydrogen until the pressure inside the reactor reached 600 psi. The reactor was heated to 285° C. and the pressure inside the vessel reached 1000 psi. The contents were stirred under these conditions for 6 h. After 6 h, contents were cooled to room temperature and filtered. The residue was transferred to a vial and N,N-dimethylacetamide was added to the vial in a 5:1 mol ratio of N,N-dimethylacetamide: terephthalic acid. The vial was warmed to 80° C. for 30 minutes to dissolve the terephthalic acid. The contents were filtered immediately; Pd on carbon was effectively removed from the terephthalic acid. Crystallized terephthalic acid filtrate was removed from the collection flask and was transferred to a clean filter where it was washed with fresh N,N-dimethylacetamide and dried. A yield of 60% purified terephthalic acid was obtained.

Example 19

Polymerization of Terephthalic Acid to Make Renewable PET

[0133] Purified terephthalic acid (PTA) obtained from Example 18 and ethylene glycol are charged to a 300 mL Parr reactor in a 1:0.9 mol ratio of PTA: ethylene glycol. Antimony (III) oxide is charged to the reactor in a 1:0.00015 mol ratio of PTA: antimony (III) oxide. The reactor is equipped with a thermocouple, mechanical stirrer, nitrogen inlet, vacuum inlet, condenser, pressure gauge, and pressure relief valve. The Parr reactor is sealed, flushed with nitrogen, heated to a temperature of 240° C., and pressurized to 4.5 bar with nitrogen. Contents are stirred under these conditions for 3 h. After 3 h, the temperature is increased to 280° C. and the system pressure is reduced to 20-30 mm by connecting the reactor to a vacuum pump. Contents are stirred under these conditions for 3 h. After 3 h, the vacuum valve is closed and the contents of the reactor are flushed with nitrogen. The reactor is opened and contents are immediately poured into cold water to form PET pellets.

Example 20

Dimerization of isobutylene to 2,5-dimethylhexenes

[0134] The product stream from Example 3 is dried over molecular sieves, compressed to 60 psig, cooled to 20° C. so that the isobutylene is condensed to a liquid, and 100 g is collected. This material is dissolved in 200 mL degassed nitrobenzene under an atmosphere of argon and charged with 10 g of the complex [η^2-isobutylene)$_2$Pd$_2$Cl$_2$(μ-Cl)$_2$] (Kharasch et al., 1938, 60, 882-884 and French Patent 1499833A). After stirring for 2 days 75% of the isobutylene is converted to 1:1 mixture of 2,5-dimethylhex-2-ene and 2,5-dimethylhex-1-ene.

Example 21

Dehydrocyclization of 2,5-dimethylhexa-2,4-diene

[0135] 2,5-dimethylhexa-2,4-diene was run neat through a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction was carried out at atmospheric pressure and a temperature of 500° C., with a WHSV of 1.0 hr^{-1}. The reactor product was condensed and analyzed by GC-MS. The reactor effluent stream was 60% xylenes, and of the xylene fraction, p-xylene was produced in greater than 99% selectivity.

Example 22

[0136] The product stream from Example 4 is dried over molecular sieves, compressed to 60 psig, cooled to 20° C. so that the isobutylene is condensed to a liquid. The isobutylene is preheated, mixed 4 parts to 1 with molecular oxygen, and then pumped into a ½ inch diameter stainless steel flow reactor packed with particles of 1:1 bismuth:antimony doped with sodium, copper, and zirconium oxides as described in Japan Patent 47-15327 and maintained at a temperature of 420° C. The flow rate of isobutylene over the catalyst in the reactor provides a catalyst contact time of ~0.45 seconds. The conversion of isobutylene is 32% with 65% selectivity towards diolefin isomers of 2,5-dimethylhexadiene.

Example 23

[0137] The 2,5-dimethylhexadiene product from Example 22 is purified by distillation and is run neat through a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction is carried out at atmospheric pressure and a temperature of 500° C., with a WHSV of 1.0 hr^{-1}. The reactor product is condensed and analyzed by GC-MS. The reactor effluent stream is 60% xylenes, and of the xylene fraction, p-xylene is produced with greater than 99% selectivity.

Example 24

[0138] The 2,5-dimethylhexene product from Example 21 is purified by distillation and is run neat through a fixed bed reactor containing a commercial chromium oxide doped alumina catalyst (BASF D-1145E ⅛"). The reaction is carried out at atmospheric pressure and a temperature of 500° C., with a WHSV of 1.0 hr^{-1}. The reactor product is condensed and analyzed by GC-MS. The reactor effluent stream is 60% xylenes, and of the xylene fraction, p-xylene is produced with greater than 99% selectivity.

We claim:

1. A method for preparing renewable p-xylene comprising:
(a) treating biomass to form a fermentation feedstock;
(b) fermenting the fermentation feedstock with one or more species of microorganism to form a fermentation broth comprising aqueous isobutanol;
(c) removing aqueous isobutanol from the fermentation broth;
(d) dehydrating, in the presence of a dehydration catalyst, at least a portion of the aqueous isobutanol of step (c), thereby forming a dehydration product comprising one or more C_4 alkenes and water;
(e) dimerizing, in the presence of an oligomerization catalyst, a dimerization feedstock comprising at least a portion of the C_4 alkenes formed in step (d), thereby forming a dimerization product comprising one or more C_8 alkenes;
(f) dehydrocyclizing, in the presence of a dehydrocyclization catalyst, a dehydrocyclization feedstock comprising at least a portion of the C_8 alkenes of step (e), thereby forming a dehydrocyclization product comprising xylenes and hydrogen, wherein the xylenes comprise at least about 75% p-xylene.

2. The method of claim **1**, wherein the dimerization product of step (e) further comprises one or more unreacted C_4 alkenes, and the dehydrocyclization product further comprises one or more unreacted C_8 alkenes, and the method further comprises:
recycling at least a portion of the unreacted C_4 alkene(s) of the dimerization product and/or the unreacted C_8 alkene(s) of the dehydrocyclization product to the dimerization feedstock of step (e); and
(ii) recycling at least a portion of the unreacted C_8 alkene(s) of the dehydrocyclization product to the dehydrocyclization feedstock of step (f).

3. The method of claim **1**, wherein at least about 95% of the one or more C_4 alkenes the dehydration product comprise isobutylene.

4. The method of claim **1**, wherein said dehydrating of step (d) is carried out in the vapor phase, thereby producing isobutylene vapor and water.

5. The method of claim **1**, wherein said dehydrating of step (d) is carried out in the liquid phase, thereby producing liquid isobutylene and water.

6. The method of claim **4**, wherein after said dehydrating of step (d), at least a portion of the water produced thereby is removed from the isobutylene vapor using a gas-liquid separator.

7. The method of claim **5**, wherein after said dehydrating step (d), a water rich phase is separated from an isobutylene rich phase using a liquid-liquid separator.

8. The method of claim **4**, wherein the isobutylene vapor is condensed prior to said dimerizing of step (e).

9. The method of claim **4**, wherein the isobutylene vapor and water are condensed after said dehydrating of step (d), prior to said dimerizing of step (e) a water rich phase is separated from an isobutylene rich phase using a liquid-liquid separator, and the dimerization feedstock comprises at least a portion of the isobutylene rich phase.

10. The method of claim **1**, further comprising adding to the dimerization feedstock of step (e) at least one diluent selected from the group consisting of t-butanol, isobutanol, water, at least one hydrocarbon, and combinations thereof.

11. The method of claim **10**, wherein the at least one diluent comprises at least one hydrocarbon, and the at least one hydrocarbon comprises at least one C_4 alkene recycled from the dimerization product of step (e) or the dehydrocyclization product of step (f), at least one C_4 alkane and/or C_8 alkane recycled from the dehydrocyclization product of step (f), or combinations thereof.

12. The method of claim **10**, wherein the diluent comprises water and isobutanol.

13. The method of claim **2**, further comprising adding to the dimerization feedstock of step (e) at least one diluent selected from the group consisting of t-butanol, isobutanol, water, at least one hydrocarbon, and combinations thereof.

14. The method of claim **13**, wherein the at least one diluent comprises at least one hydrocarbon, and the at least one hydrocarbon comprises at least one C_4 alkene recycled from step (e) or step (f), at least one C_4 alkane and/or C_8 alkane recycled from step (f), or combinations thereof.

15. The method of claim **1**, wherein the at least one or more C_8 alkenes of the dimerization product comprises about 50-100% of 2,4,4-trimethylpentenes.

16. The method of claim **15**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 75% of 2,4,4-trimethylpentenes.

17. The method of claim **15**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 90% of 2,4,4-trimethylpentenes.

18. The method of claim **1**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 50-100% of 2,5-dimethylhexene.

19. The method of claim **18**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 75% of 2,5-dimethylhexene.

20. The method of claim **18**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 90% of 2,5-dimethylhexene.

21. The method of claim **1**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 50-100% of 2,5-dimethylhexadiene.

22. The method of claim **21**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 75% of 2,5-dimethylhexadiene.

23. The method of claim **21**, wherein the at least one or more C_8 alkenes of the dimerization product comprises at least about 90% of 2,5-dimethylhexadiene.

24. The method of claim **1**, further comprising adding to the dehydrocyclization feedstock of step (f) at least one diluent selected from the group consisting of nitrogen, argon, methane, isobutylene, isobutane, isooctane, light aromatics, and combinations thereof.

25. The method of claim **24**, wherein the at least one diluent comprises isobutylene, which is unreacted isobutylene from steps (e) and/or (f), or a byproduct from step (f).

26. The method of claim **1**, wherein:

said dehydrocyclization of step (f) is carried out at a conversion of less than about 100%; and

unreacted C_8 alkenes are recycled back to the dehydrocyclization feedstock of step (f).

27. The method of claim **1**, wherein steps (e) and (f) are carried out simultaneously.

28. The method of claim **1**, wherein steps (e) and (f) are carried out sequentially.

29. The method of claim **1**, wherein the xylenes of the dehydrocyclization product comprise at least about 90% p-xylene.

30. The method of claim **1**, wherein said dehydrating is carried out at temperature of at least about 100° C. and a pressure of at least about 1 atm.

31. The method of claim **1**, wherein the dehydration catalyst is an organic or inorganic acid, or a metal salt thereof.

32. The method of claim **26**, wherein the dehydration catalyst is a heterogeneous acidic γ-alumina catalyst.

33. The method of claim **1**, wherein the oligomerization catalyst is a heterogeneous acidic catalyst.

34. The method of claim **33**, wherein the oligomerization catalyst is an acidic zeolite, solid phosphoric acid, or a sulfonic acid resin.

35. The method of claim **1**, wherein the dehydrocyclization catalyst is a heterogeneous metal-containing dehydrogenation catalyst.

36. The method of claim **35**, wherein the dehydrocyclization catalyst is a supported chromium-containing compound.

37. The method of claim **33**, wherein the dehydrocyclization catalyst is selected from the group consisting of chromium-oxide treated alumina; platinum- and tin-containing zeolites; and alumina, cobalt- or molybdenum-containing alumina.

38. The method of claim **1**, wherein the aqueous isobutanol removed in step (c) consists essentially of isobutanol and 0-15% water.

39. The method of claim **1**, further comprising hydrogenating an alkene in the presence of dehydrogenation catalyst with the hydrogen from step (f).

40. The method of claim **27**, wherein said steps (e) and (f) are carried out simultaneously under oxidizing conditions.

41. The method of claim **40**, wherein steps (e) and (f) are carried out in the presence of a single catalyst comprising bismuth oxide.

42. The method of claim **41**, wherein the C_4 alkenes comprise isobutylene.

43. A method of preparing renewable terephthalic acid comprising:

preparing renewable p-xylene by the method of claim **1**, then oxidizing the p-xylene in the presence of an oxidizing agent, thereby forming renewable terephthalic acid.

44. The method of claim **43**, wherein the oxidizing agent comprises an oxidation catalyst and oxygen.

45. A method of preparing a renewable polyester comprising:

reacting renewable terephthalic acid prepared by the method of claim **40** with ethylene glycol or butylene glycol in the presence of an acidic polymerization catalyst.

46. The method of claim **45**, wherein the acidic polymerization catalyst is antimony (III) oxide.

47. The method of claim **45**, wherein the polyester is polyethylene terephthalate, and the ethylene glycol is renewable ethylene glycol.

48. The method of claim **45**, wherein the polyester is polypropylene terephthalate, and the propylene glycol is renewable propylene glycol.

49. The method of claim **1**, further comprising hydrogenating a portion of the dimerization product with at least a portion of the hydrogen of the dehydrocyclization product.

* * * * *

Section 25.3
Equipment Design Calculations

Section 25.3.1: Calculations for Pressure Changers

Equations are taken from Seider et. al. Chapter 16, Section 5, Pages 451-456.

Pump sample calculation shown for P-201

$$Head = \frac{Pressure\ Change}{Fluid\ Density}\ \frac{\Delta P}{\rho} = \frac{20\ psig * 144\ \frac{in^2}{ft^2}}{34.4\ \frac{lb}{ft^3}} = 83.7\ ft$$

$$Pump\ Efficiency = \eta_P = -0.316 + 0.24015(lnQ) - 0.01199(lnQ)^2$$
$$= -0.316 + 0.24015(\ln(3244\ gpm)) - 0.01199(\ln(3244\ gpm))^2 = 0.842$$

$$Pump\ Brake\ Horsepower = P_B = \frac{QH\rho}{33{,}000 * \eta_P} = \frac{3244\ gpm * 83.7\ ft *\ 4.6\ \frac{lb}{gal}}{33{,}000 * 0.842}$$
$$= 45\ BHp$$

$$Motor\ Efficiency = n_m = 0.80 + 0.0319(lnP_B) - 0.01182(lnP_B)^2$$
$$= 0.80 + 0.0319(\ln(45\ BHp)) - 0.01182(\ln(45(BHp)))^2 = 0.895$$

$$Power\ Consumption = P_C = \frac{P_B}{n_m} = \frac{45\ BHp}{0.895} * \frac{0.7457\ kW}{hp} * 1\ hr = 37.3\ kWh$$

The volumetric flow rate from ASPEN and the head from the calculation were used in Table 16.20 to obtain other data for the type of pump.

Compressor sample calculation shown for C-501

Compressors follow above calculations with additional need to calculate the compression ratio to determine the number of stages.

$$Compression\ Ratio = \frac{Outlet\ Pressure}{Inlet\ Pressure} = \frac{285\ psig}{24\ psig} = 11.88$$

The compression ratio should be no larger than 3; therefore, this compressor needs multiple stages with intercoolers in between.

Section 25.3.2: Calculations for Heat Exchangers

Equations are taken from Seider et. al. Chapter 12 and from UPenn CBE460 Class Handouts.

Heat Exchanger sample calculation shown for E-201

Heat transfer coefficient obtained from Table 12.5 depending on the two fluids used.

$$\Delta T_1 = \Delta T_{hot,in} - \Delta T_{cold,out} = 372 - 105 = 267ºF$$

$$\Delta T_2 = \Delta T_{hot,out} - \Delta T_{cold,in} = 300 - 80 = 220ºF$$

$$Log\ Mean\ Tempreature\ Difference = \Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} = \frac{267 - 220}{\ln\left(\frac{267}{220}\right)} = 242.7ºF$$

Assume the correction factor, F_T, = 1

$$Area = A_i = \frac{Q}{U * \Delta T_{lm} * F_T} = \frac{45{,}923{,}350\ BTU/hr}{100\frac{BTU}{ºF * ft^2 * hr} * 242.7ºF * 1} = 1{,}891.9\ ft^2$$

A tube velocity was chosen between 1 and 10 ft/sec to obtain a reasonable number of tube passes.

$$Cross - sectional\ area\ per\ pass = A_c = \frac{tube\ flow\ rate}{\rho * tube\ velocity} = \frac{1{,}826{,}975\frac{lb}{hr}}{62\ \frac{lb}{ft^3} * 8\frac{ft}{s} * 3600\frac{s}{hr}}$$

$$= 1.03\ ft^2$$

Assume inner diameter of tube, D_i, is 1 inch (0.083 ft).

$$No. of\ tubes\ per\ pass = N_t = \frac{4 * A_c}{\pi * D_i^2} = \frac{4 * 1.03\ ft^2}{\pi * (0.083\ ft)^2} = 188.6$$

Round N_t to a whole number.

A tube length was chosen between 20 and 30 ft to obtain a reasonable number of passes.

$$Heat\ transfer\ area\ per\ tube = A_t = \pi * D_i * L = \pi * (0.083\ ft) * (24\ ft) = 6.28\ ft^2$$

$$No. of\ tube\ passes = N_p = \frac{A_i}{A_t * N_t} = \frac{1891.9\ ft^2}{6.28\ ft^2 * 189} = 1.59$$

Round N_p to a whole number.

Calculate new A_t from rounded numbers.

$$A_t = \frac{A_i}{N_p * N_t} = \frac{1891.9\, ft^2}{2 * 189} = 5.0\, ft^2$$

Get new L from new A_t.

$$L = \frac{A_t}{\pi * D_i} = \frac{5.0\, ft^2}{\pi * 0.083\, ft} = 19.1\, ft$$

Get new A_i from new L.

$$A_i = \pi * L * D_i * N_p * N_t = \pi * 19.1\, ft * 0.083\, ft * 2 * 189 = 1{,}891.9\, ft^2$$

Obtain shell diameter from Table 12.6 using $N_p * N_t = 2 * 189 = 378$. Therefore, the shell diameter for a heat exchanger with a square pitch, 1 in O.D. tubes, and two passes is 31 inches.

$$Baffle\ spacing = b\text{:}\ \frac{D_s}{5} < b < D_s = 7.4 < b < 37.\ b \sim 22.2\ inches$$

If process stream is being cooled (by cooling or chilled water):

$$Utility\ mass\ flow\ rate = m = \frac{Q\ BTU/hr}{C_p\ \frac{BTU}{lb * ºF} * \Delta T\ ºF}$$

If process stream is being heated (by steam):

$$Utility\ mass\ flow\ rate = m = \frac{Q\ BTU/hr}{\Delta H_{vap}\ \frac{BTU}{lb}}$$

Section 25.3.3: Reactors and Amount of Catalyst

Equations are taken from Seider et. al. Chapter 15 and Chapter 16.

Reactor sample calculation shown for R-201

WHSV was obtained from the patent.

$$Mass\ of\ catalyst = \frac{mass\ flow\ rate\ of\ reactor\ feed}{WHSV} = \frac{1{,}077{,}140\ lb/hr}{15\ hr^{-1}} = 71{,}809\ lb$$

$$Volume\ of\ catayst = \frac{mass\ of\ catalyst}{bulk\ density\ of\ catalyst} = \frac{71809\ lb}{45.26\ \frac{lb}{ft^3}} = 1{,}587\ ft^3$$

$$Volume\ of\ reactor = vol\ of\ catalyst * 10\%\ safety\ factor = 1587 * 1.1 = 1{,}745\ ft^3$$

$$Reactor\ residence\ time = \frac{volume\ of\ reactor}{volumetric\ flow\ rate\ of\ reactor\ feed} = \frac{1745\ ft^3}{30479 \frac{ft^3}{hr} * \frac{1\ hr}{60\ min}}$$

$$= 3.44 \min = 206\ sec$$

Assume an L/D aspect ratio of 4.

$$Diameter = \left(\frac{4 * V}{\pi * \frac{L}{D}}\right)^{\frac{1}{3}} = \left(\frac{4 * 1745}{\pi * 4}\right)^{\frac{1}{3}} = 8.2\ ft$$

$$Height = \frac{L}{D} * D = 4 * 8.2\ ft = 32.9\ ft$$

$$Cross - sectional\ area = \frac{\pi * D^2}{4} = \frac{\pi * (8.2\ ft)^2}{4} = 53.1\ ft^2$$

$$Superficial\ fluid\ velocity = \frac{volumetric\ flow\ rate}{cross - sect\ area} = \frac{30479 \frac{ft^3}{hr} * \frac{1\ hr}{3600\ s}}{53.1\ ft^2} = 0.16\ ft/s$$

Section 25.3.4: Distillation Columns

ASPEN was used to calculate the number of trays, the tray diameter, and the number of passes. The O'Connel Correlation was used to obtain the optimal number of trays, the optimal location of the feed tray, and the tray efficiencies. The relative volatilities and liquid viscosities of the materials were taken from ASPEN. The following calculations were done.

$$Relative\ volatility = \frac{K_1}{K_2}$$

$$Stage\ Efficiecy = 0.492 * (relative\ volatility * viscosity)^{-0.245}$$

$$Real\ Trays\ Required = \frac{1}{Stage\ Efficiency}$$

These values were calculated, and the results are shown in Table 25.3.1 and Table 25.3.1 for S-301 and S-501, respectively. For S-301 separating out the trimers, the correlation shows that the number of trays should be 17 instead of 9, and that the feed tray should be on stage 11 and not stage 6, with an average tray efficiency of 0.44. For S-501 separating out p-xylene and hydrogen, the correlation shows that the number of trays should be 23 instead of 16 for S-301, and that the feed tray should be on stage 8 and not stage 5, with an average tray efficiency of 0.62.

Table 25.3.1 Data from the O'Connel Correlation for S-301. The bolded numbers are the total number of trays and the actual feed tray.

ASPEN Theoretical Tray Number	**Viscosity of Liquid from Stage (Centipose)**	**K_2 VALUE Trimers**	**K_1 VALUE TMP**	**Relative Volatility**	**Stage Efficiency**	**Real Trays Required**	**Real Tray Number**
Condenser 1	0.1633	0.0093	0.3018	32.3540			Condenser
2	0.1250	0.0669	1.0108	15.1029	0.42	2.37	2.37
3	0.1310	0.0802	1.1331	14.1203	0.42	2.36	4.74
4	0.1357	0.0936	1.2487	13.3464	0.43	2.35	7.09
5	0.1376	0.1005	1.3067	12.9971	0.43	2.34	9.43
6	0.1381	0.1030	1.3263	12.8777	0.43	2.34	**11.77**
7	0.1455	0.2043	2.0747	10.1540	0.45	2.24	14.01
8	0.1397	0.5209	4.0038	7.6863	0.48	2.07	**16.08**
Reboiler 9	0.1322	0.8555	5.8958	6.8919			Reboiler

Table 25.3.2 Data from the O'Connel Correlation for S-501. The bolded numbers are the total number of trays and the actual feed tray.

ASPEN Theoretical Tray Number	**Viscosity of Liquid from Stage (Centipose)**	**K_2 VALUE p-Xylene**	**K_1 VALUE TMP**	**Relative Volatility**	**Stage Efficiency**	**Real Trays Required**	**Real Tray Number**
Condenser 1	0.3828	0.0088	0.0400	4.5685			Condenser
2	0.1887	0.2136	0.5795	2.7129	0.58	1.72	1.72
3	0.1806	0.2757	0.7171	2.6016	0.59	1.69	3.41
4	0.1816	0.3146	0.8007	2.5452	0.59	1.68	5.10
5	0.1839	0.3738	0.9248	2.4739	0.60	1.68	6.77
6	0.1654	0.6248	1.4230	2.2773	0.62	1.60	**8.37**
7	0.1659	0.7116	1.5871	2.2302	0.63	1.59	9.97
8	0.1662	0.8013	1.7536	2.1885	0.63	1.59	11.55
9	0.1664	0.8767	1.8915	2.1576	0.63	1.58	13.13
10	0.1665	0.9301	1.9879	2.1374	0.63	1.58	14.71
11	0.1665	0.9636	2.0477	2.1251	0.63	1.58	16.29
12	0.1665	0.9832	2.0822	2.1179	0.64	1.57	17.86
13	0.1665	0.9942	2.1012	2.1135	0.64	1.57	19.44
14	0.1664	1.0005	2.1117	2.1106	0.64	1.57	21.01
15	0.1664	1.0047	2.1184	2.1085	0.64	1.57	**22.58**
Reboiler 16	0.1665	1.0110	2.1288	2.1057			Reboiler

Using the number of trays from the O'Connel correlation, the height of the columns was calculated. According to common practice, the tray spacing is 2 ft, the headspace is 4 ft, the sumpspace is 10 ft, the feed location spacing is 3 ft, and the disengaging space is 3 ft.

$$Height = space\ between\ trays + headspace + sumpspace + feed\ location\ spacing + disengaging\ space$$

$$S301\ Height = \left(3 * (17 - 1)\right) + 4 + 10 + 3 + 3 = 52\ ft$$

$$S501\ Height = \left(3 * (23 - 1)\right) + 4 + 10 + 3 + 3 = 64\ ft$$

The other parts of the distillation column were modeled by calculations show in the other sections. The reflux pumps were calculated using equations in Section 25.3.1. The reflux accumulators were calculated using the equations for the diameter and height in Section 25.5.3, with an additional multiplication of a residence time of 5 minutes. The reboilers and condensers were designed using calculations in Section 25.3.2.

Section 25.3.5: Flash Drum

Equations are taken from *Chemical Engineering Process Design and Economics.*[27]

Flash Drum sample calculation shown for S-502

Assume a hold-up time of 10 minutes according to the textbook stated above.

$$Volume\ of\ Liquid\ Held = volumetric\ flow\ rate * molar\ liquid\ fraction * holdup\ time$$
$$= 271\ \frac{ft^3}{hr} * 0.05 * \frac{10\ min}{60\ min/hr} = \ 2.26\ ft^3$$

Assume liquid level in the tank will be 50% according to the textbook stated above. Assume an L/D ratio of 3.

$$Diameter = (\frac{4 * V}{\pi * \frac{L}{D} * level\ in\ tank})^{\frac{1}{3}} = \ (\frac{4 * 2.26\ ft^3}{\pi * 3 * 0.5})^{\frac{1}{3}} = 1.2\ ft$$

$$Height = \frac{L}{D} * D = 3 * 1.2\ ft = 3.7\ ft$$

The tank is very small due to the fact that the molar vapor fraction is very large at 95%. Other calculations may be more accurate by using the vapor velocity to prevent entrainment of fluid. While the above dimensions were used for the project, the equations below show other calculations from the textbook listed above. A maximum allowed vapor velocity is calculated to let 100 um droplets fall.

$$Maximum\ allowed\ vapor\ velocity = 0.21\frac{ft}{s} * \left(\frac{liq\ density - vapor\ density}{vapor\ density}\right)^{0.5}$$
$$= 0.21\frac{ft}{s} * \left(\frac{43.9\ \frac{lb}{ft^3} - 0.149\ \frac{lb}{ft^3}}{0.149\ \frac{lb}{ft^3}}\right)^{0.5} = 3.6\ ft/s$$

$$Cross\ sectional\ area\ when\ the\ tank\ is\ half\ full = \pi * r^2 = \pi * 0.6^2 = 1.89\ ft^2$$

$$Actual\ vapor\ velocity = \frac{volumetric\ flow\ rate}{cross - sectional\ area} = \frac{271\ \frac{ft^3}{hr} * \frac{1\ hr}{3600\ s}}{1.89\ ft^2} = 0.04\ ft/s$$

Because the vapor velocity is less than the maximum allowed vapor velocity, the tank does not need to be larger than the dimensions calculated above.

Section 25.3.6: Storage and Surge Tanks

Equations are taken from Seider et. al. Chapter 16.

Tank sample calculation shown for T-102

Time capacity is the amount of time the material will be stored.

Assume a safety factor of 1.5.

$$Volume\ of\ Tank = volumetric\ flow\ rate * time\ capacity * safety\ factor$$
$$= 10.34\ \frac{ft^3}{hr} * 504\ hr * 1.5 = 7{,}820\ ft^3 = 59{,}277\ gal$$

Assume an L/D ratio of 3.

$$Diameter = \left(\frac{4 * V}{\pi * \frac{L}{D}}\right)^{\frac{1}{3}} = 14.9\ ft$$

$$Height = \frac{L}{D} * D = 4 * 8.2\ ft = 44.8\ ft$$

$$Surface\ area = (2 * \pi * r^2) + (2 * \pi * r * L) = (2 * \pi * 7.45^2) + (2 * \pi * 7.45 * 44.8)$$
$$= 2{,}447\ ft^2$$

Determine what type of tank will be used and find the cost equation in Table 16.32 on pg. 485.

Floating roof: $C_p = 475 * V^{0.507} = 475 * (59277\ gal)^{0.507} = \$124{,}896$

Cone roof: $C_p = 265 * V^{0.513}$

Section 25.3.7: Catalyst Regeneration Utility Calculation for R-401

We are assuming all of the coke is pure carbon deposits.

$$Mass\ of\ catalyst\ per\ reactor = \frac{mass\ flow\ rate\ of\ reactor\ feed\ per\ reactor}{WHSV}$$
$$= \frac{536{,}716\ lb/hr}{1.1\ hr^{-1}} = 487{,}924\ lb$$

According to industry experts, the extent of coking will be 7%.

$$Mass\ of\ coke = mass\ of\ catalyst * extent\ of\ coking = 487925\ lb * \ 0.07 = 34{,}155\ lb$$

$$Moles\ of\ coke = \frac{mass\ of\ coke}{molecular\ weight\ of\ carbon} = \frac{34155\ lb}{12\ lb/lbmol} = 2{,}846\ lbmol$$

Combustion reaction: $C + O_2 \rightarrow CO_2$

$$Moles\ of\ O_2 = 2846\ lbmol\ C * \frac{1\ lbmol\ O_2}{1\ lbmol\ C} = 2846\ lbmol\ O_2$$

$$Mole\ flow\ rate\ of\ oxygen\ during\ process = \frac{moles\ of O_2}{burn\ time} = \frac{2846\ lbmol}{8\ hrs}$$
$$= 365\ lbmol/hr$$

$$Mass\ flow\ rate\ of\ O_2 = \ 365\frac{lbmol}{hr} * \frac{32\ lb}{lbmol} = 11{,}385\ lb/hr$$

Initial feed for decoking process will be 1% oxygen.

$$Total\ flow\ rate\ for\ process = \frac{mass\ flow\ rate\ of\ oxygen}{0.01} = 1{,}138{,}489\ lb/hr$$

Initial feed for decoking process must be 95 parts nitrogen and 5 parts air.

$$Nitrogen\ flow\ rate = total\ flow\ rate * \ 0.95 = \ 1{,}081{,}565\ lb/hr$$

$$Amt\ of\ Nitrogen\ needed\ for\ whole\ process = flow\ rate * burning\ time = 8{,}652{,}519\ lbs$$

$$Air\ flow\ rate = total\ flow\ rate * \ 0.05 = \ 56{,}924\ lb/hr$$

$$Amt\ of\ Air\ needed\ for\ whole\ process = flow\ rate * burning\ time = 455{,}396\ lbs$$

After first pass of decoking, effluent will be recycled back around. Therefore, pure nitrogen will only need to make up 10 parts of the stream.

$$Nitrogen\ flow\ rate = total\ flow\ rate * \ 0.10 = \ 113{,}849\ lb/hr$$

$$Amt\ of\ Nitrogen\ needed\ for\ whole\ process = flow\ rate * burning\ time = 910{,}791\ lbs$$

The decoking process will occur every 5 days. Therefore, it will occur 94 times a year. During the 1st time, the stream will be 95 parts pure nitrogen and 5 parts pure air. The other 93 times, the stream will be 10 parts pure nitrogen, 5 parts pure air, and 85 parts recycle.

$$\begin{aligned} Total\ Amt\ of\ Nitrogen\ needed\ for\ all\ decoking &= (8652519 * 1) + (910791 * 93) \\ &= 92{,}991{,}809\ lb \end{aligned}$$

$$Total\ Amt\ of\ Air\ needed\ for\ all\ decoking = 455{,}396 * 94 = 42{,}807{,}224\ lb$$

Section 25.4
MSDS

Safety Data Sheet

1 IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY

Product name	Isobutene (Isobutylene)
Chemical formula	$(CH_3)_2C=CH_2$
Company identification	see heading and/or footer
Emergency phone numbers	see heading and/or footer

2 COMPOSITION/INFORMATION ON INGREDIENTS

Substance/Preparation	Substance.
Components/Impurities	Contains no other components or impurities which will influence the classification of the product.
CAS Nr	00115-11-7
EC Nr (from EINECS)	204-066-3

3 HAZARDS IDENTIFICATION

Hazards identification	Liquefied gas Extremely flammable

4 FIRST AID MEASURES

Inhalation	In low concentrations may cause narcotic effects. Symptoms may include dizziness, headache, nausea and loss of co-ordination. In high concentrations may cause asphyxiation. Symptoms may include loss of mobility/consciousness. Victim may not be aware of asphyxiation. 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	In case of frostbite spray with water for at least 15 minutes. Apply a sterile dressing. Immediately flush eyes thoroughly 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 away from the container and 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.

7 HANDLING AND STORAGE

Handling and storage	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). Segregate from oxidant gases and other oxidants in store. Refer to supplier's container handling instructions. Keep container below 50°C in a well ventilated place.

8 EXPOSURE CONTROLS/PERSONAL PROTECTION

Personal protection	Ensure adequate ventilation. Do not smoke while handling product.

9 PHYSICAL AND CHEMICAL PROPERTIES

Molecular weight	56
Melting point	-140.4 °C
Boiling point	-6.9 °C

Critical temperature	145 °C
Relative density, gas	1.9 (air=1)
Relative density, liquid	0.63 (water=1)
Vapour Pressure 20°C	2.6 bar
Solubility mg/l water	388 mg/l
Appearance/Colour	Colourless gas
Odour	Sweetish Poor warning properties at low concentrations.
Autoignition temperature	465 °C
Flammability range	1.6-10 vol% in air.
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

General	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.

14 TRANSPORT INFORMATION

UN Nr	1055
Class	2.1
ADR/RID Classification code	2F
ADR/RID Hazard Nr	23
Labelling ADR	Label 2.1: flammable gas

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 and: - cylinder valve is closed and not leaking - valve outlet cap nut or plug (where provided) is correctly fitted - valve protection device (where provided) is correctly fitted - there is adequate ventilation. - compliance with applicable regulations.

15 REGULATORY INFORMATION

Number in Annex I of Dir 67/548	Not included in Annex I.
EC Classification	F+;R12
-Symbols	F+: Extremely flammable
Labelling of cylinders	
-Symbols	Label 2.1: flammable gas
-Risk phrases	R12 Extremely flammable.
-Safety phrases	S9 Keep container in well ventilated place. S16 Keep away from ignition sources - No smoking. S33 Take precautionary measures against static discharges.

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.

Users of breathing apparatus must be trained.

Before using this product in any new process or experiment, a thorough material compatibility and safety study should be carried out.

Details given in this document are believed to be correct at the time of going to press. 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.

End of document.
Number of pages :4

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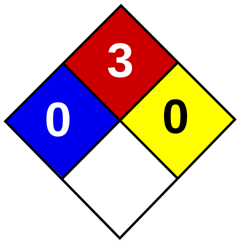

Health	2
Fire	3
Reactivity	0
Personal Protection	J

Material Safety Data Sheet
2,2,4-trimethylpentane MSDS

Section 1: Chemical Product and Company Identification

Product Name: 2,2,4-trimethylpentane

Catalog Codes: SLT3712

CAS#: 540-84-1

RTECS: SA3320000

TSCA: TSCA 8(b) inventory: 2,2,4-trimethylpentane

CI#: Not available.

Synonym: Isooctane; Isobutyltrimethylpentane

Chemical Name: 2,2,4-Trimethylpentane

Chemical Formula: C8H18

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
{2,2,4-}trimethylpentane	540-84-1	100

Toxicological Data on Ingredients: 2,2,4-trimethylpentane LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

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

Potential Chronic Health Effects:
Slightly hazardous in case of skin contact (sensitizer). CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to eyes. The substance may be toxic to kidneys, lungs, liver, skin, central nervous system (CNS). 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. 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. 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: Not available.

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

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

Ingestion:
If swallowed, do NOT induce vomiting. Never give anything by mouth to an unconscious person. Aspiration hazard if swallowed- can enter lungs and cause damage. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 418°C (784.4°F)

Flash Points: CLOSED CUP: -12°C (10.4°F). OPEN CUP: 4.5°C (40.1°F).

Flammable Limits: LOWER: 1.1% UPPER: 6%

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. 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. Slightly explosive in presence 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: Vapor may travel considerable distance to source of ignition and flash back.

Special Remarks on Explosion Hazards: May form explosive mixtures with air.

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. Call for assistance on disposal.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not breathe gas/ fumes/ vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If you feel unwell, seek medical attention and show the label when possible. Keep away from incompatibles such as oxidizing agents, reducing agents, acids, alkalis.

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

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.

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: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Benzene-like. Odor of gasoline

Taste: Not available.

Molecular Weight: 114.23 g/mole

Color: Colorless. Clear

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

Boiling Point: 99.238°C (210.6°F)

Melting Point: -107.45°C (-161.4°F)

Critical Temperature: Not available.

Specific Gravity: 0.69194 (Water = 1)

Vapor Pressure: 5.4 kPa (@ 20°C)

Vapor Density: 3.93 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

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

Solubility:
Soluble in diethyl ether, acetone. Insoluble in cold water Somewhat soluble in absolute alcohol. Soluble in Benzene, Toluene, Xylene, Chloroform, Carbon Disulfide, Carbon Tetrachloride.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

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

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

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

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

Toxicity to Animals:
LD50: Not available. LC50: Not available.

Chronic Effects on Humans:
Causes damage to the following organs: eyes. May cause damage to the following organs: kidneys, lungs, liver, skin, central nervous system (CNS).

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: May affect genetic material (mutagenic)

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: May cause skin irritation. It is not known whether it enters the body through the skin. Eyes: Causes eye irritation. Inhalation: May cause irritation of the respiratory tract (nose, throat and lungs) with coughing, wheezing, shortness of breath, and pulmonary edema. Higher levels could cause "chemical pneumonia" and may cause you to pass out and even stop breathing. May affect behavior/central nervous system and cause narcotic effects at high concentration (CNS depression - dizziness, drowsiness, lightheadedness, poor coordination, reduced alertness, headache, unconciousness, coma) and cause nausea. Ingestion: May cause gastrointestinal tract irritation with nausea, vomiting, and diarrhea. May affect behavior/central nervous system (CNS depression with symptoms similar to that of inhalation) Chronic Potential Health Effects: Skin: Prolonged or repeated exposure may cause defatting of the skin and dermatitis. Ingestion: Prolonged or repeated ingestion may affect the kidneys, and liver.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

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

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

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

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Octane UNNA: 1262 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: 2,2,4-trimethylpentane Florida: 2,2,4-trimethylpentane Massachusetts RTK: 2,2,4-trimethylpentane New Jersey: 2,2,4-trimethylpentane TSCA 8(b) inventory: 2,2,4-trimethylpentane TSCA 8(d) H and S data reporting: 2,2,4-trimethylpentane: 12/19/95 CERCLA: Hazardous substances.: 2,2,4-trimethylpentane: 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-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R11- Highly flammable. R38- Irritating to skin. R50- Very toxic to aquatic organisms. R65- Harmful: may cause lung damage if swallowed. S2- Keep out of the reach of children. S9- Keep container in a well-ventilated place. S16- Keep away from sources of ignition - No smoking. S29- Do not empty into drains. S33- Take precautionary measures against static discharges. S60- This material and its container must be disposed of as hazardous waste. S61- Avoid release to the environment. Refer to special instructions/Safety data sheets. S62- If swallowed, do not induce vomiting: seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: j

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

Health: 0

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Not applicable. 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 08:55 PM

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

GELEST, INC.

11 East Steel Rd. Morrisville, PA 19067
Phone: (215) 547-1015

MATERIAL SAFETY
DATA SHEET

EMERGENCY TELEPHONE
CHEMTREC: 1-800-424-9300

NAME USED ON LABEL: **ISOOCTENE - ENEI1470**
CHEMICAL NAME: ISOOCTENE
SYNONYMS: DIISOBUTYLENE; 2,4,4-TRIMETHYLPENTENE
CHEMICAL FAMILY: HYDROCARBON
FORMULA: C_8H_{16}
HMIS CODES HEALTH: 1 FLAMMABILITY: 3 REACTIVITY: 0

INGREDIENTS

IDENTITY	CAS NO.	%	TLV	OSHA PEL
2,4,4-TRIMETHYLPENTENE-1	107-39-1	>75	5mg/m^3(8H)	not established
2,4,4-TRIMETHYLPENTENE-2	107-40-4	<25	not established	not established

PHYSICAL DATA

Boiling Point: 101-104°C
Specific Gravity: 0.717
Vapor Density (air = 1): 4
% volatiles: 100
Molecular Weight: 112.21

Melting Point: < -100°C
Vapor Pressure, 25°: 43.4mm
Solubility in water: insoluble (1.8mg/l)
Evaporation rate (butyl acetate = 1): ~1
Refractive Index: 1.408

Appearance & Color: clear liquid with strong odor

FIRE & EXPLOSION DATA

Flash Point, CC: -4°C (25°F)
Autoignition Temp.: 380°
Flammability Limits- LEL: 1% UEL: 7%

Extinguishing Media: Water spray or fog, foam, carbon dioxide, dry chemical.
Special Fire Fighting Procedures: Avoid eye and skin contact. Do not breathe fumes or inhale vapors.
Unusual Fire and Explosion Hazards: Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

ENVIRONMENTAL INFORMATION

Spill response: Sweep material and transfer to a suitable container for disposal.

Recommended Disposal: Incinerate. Follow all chemical pollution control regulations.

Toxicity to daphnia, LC50: 1.2 mg/l (48H)

HEALTH HAZARD DATA

Eye Contact: May cause immediate or delayed severe eye irritation.

Skin contact: May cause mild skin irritation. Avoid Contact.

Inhalation: No information available. Avoid inhalation.

Oral Toxicity- rat, LD50: >12,500mg/kg
Inhalation Toxicity- rat, LC50: >4900ppm/20H
Chronic Toxicity: No animal results. Ames test (histidine reversion) is negative, i.e not a mutagen.

SUGGESTED FIRST AID

EYES: In case of contact, immediately flush eyes with flowing water for at least 15 minutes. Get medical attention.

SKIN: Flush with water, then wash with soap and water.

INHALATION: Move exposed individual to fresh air. Administer oxygen if needed. Call a physician.

INGESTION: Never give fluids or induce vomiting if patient is unconscious or having convulsions. To conscious individual give one full cup of water to dilute ingested material. Get medical attention.

REACTIVITY DATA

Stability: Stable
Conditions to avoid: Store away from oxidizers.
Hazardous decomposition products: Organic acid vapors..

SPECIAL PROTECTION INFORMATION

Ventilation: Local exhaust is recommended. Mechanical is recommended.
Respiratory Protection: If exposure exceeds TLV, NIOSH approved organic vapor respirator.
Eye and Face Protection: Chemical worker’s goggles. Do not wear contact lenses.
Other Clothing and Equipment: Rubber, neoprene or nitrile gloves. An eyewash and emergency shower should be available. Launder clothing before reuse.

OTHER PRECAUTIONS

For research and industrial use only.

Storage and Handling: Store in sealed containers.

TRANSPORTATION

DOT SHIPPING NAME: DIISOBUTYLENE, ISOMERIC COMPOUNDS
DOT HAZARD CLASS: 3
DOT LABEL: Flammable Liquid
DOT ID No: 2050 PG: II ERG: 3L

Prepared by safety and environmental affairs MSDS ISSUE DATE ENEI1470: 10/16/14
SUPERSEDES: none

Technical information

GPS Safety Summary

Tributene

Substance name

Tributene

CAS-No. 97280-83-6

General Statement

Tributene is an olefinic hydrocarbon consisting of branched C12 olefin isomers. It is a low molecular weight liquid of moderate volatility.
Tributene is used as an intermediate for the production of other chemicals or as a fuel component. Because it is used as an intermediate in chemical industry or burnt as a fuel with limited concentration in the fuel exposure is very limited.

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Chemical identity

Name	Tributene
Brand names	Tributene
Chemical name (IUPAC)	Isododecene
CAS number	97280-83-6
Molecular formula	$C_{12}H_{24}$
Chemical characterization	Branched C12 olefin mixture

Uses and application

It is used as an intermediate for the production of other chemicals or as a fuel component.

Physical/chemical properies

Tributene is a low molecular weight liquid of moderate volatility.
The liquid is lighter than water, only very slightly soluble in water, while vapors are heavier than air.

Property	Value
Physical state	Liquid
Color	Colorless
Odor	Odorless
Density	0,77 g/cm3 (20 °C) Vapour heavier than air
Melting / boiling point	<-150 °C / 118 - 132 °C (1013 hPa)
Flammability	highly flammable liquid flammability limits 0.3% (V) - 7.5% (V)
Explosive Properties	No explosive properties
Self-ignition temperature	210 °C
Vapor pressure	9 hPa (20 °C)
Molecular weight	168 g/mol
Water solubility	<2.4 mg/l
Flash point	71 °C Method: closed cup
Octanol-water partition coefficient	log Pow: 7.6-7.8

Health effects

Effect Assessment	Result
Acute toxicity (oral, dermal and inhalation)	Low acute toxicity. Inhalation of high vapor concentrations can cause CNS-depression and narcosis. Harmful: May cause lung damage if swallowed.
Eye / Skin irritation	Moderately irritating to the skin but not eye irritating.
Sensitization	Not considered to be sensitizing.
Toxicity after repeated exposure	Target organ effects specific to rodents are not relevant to human health
Genotoxicity/mutagenicity	Not mutagenic / genotoxic
Carcinogenicity	No data but based on chemical structure not considered to be a human cancer concern
Toxicity for reproduction	No adverse effects on fertility and not

	selectively toxic to the fetus (derived from test results with similar substances)

Environmental effects

Effect Assessment	Result
Aquatic toxicity	Not toxic to water organisms in the range of water solubility.

Fate and Behavior	Result
Biodegradation	Biodegradable
Bioaccumulation potential	Bioaccumulation possible
PBT / vPvB conclusion	Neither considered to be PBT nor vPvB

Photochemical degradation takes place.

Exposure

Human health

Because the substance is handled in closed systems under controlled conditions and is contained in public used products only in minor concentrations (e.g. in fuel) , no relevant exposure is to be expected.

Environment

Because the substance is handled in closed systems under controlled conditions and is contained in public used products only in minor concentrations (e.g. in fuel) , no relevant exposure is to be expected.

Risk management recommendations

Industry use, production and formulation

- Assumes a good basic standard of occupational hygiene is implemented
- Substance is handled in closed systems under controlled conditions only.
- Avoid contact with skin and eyes.
- Do not inhale vapor, aerosols, mist.
- Ensure adequate ventilation.
- Take precautionary measures against static charges, keep away from sources of ignition.
- Wear personal protective equipment
    - Chemical-resistant protective gloves (EN 374)
      Glove material nitrile-butadiene rubber (NBR) gloves
    - Protective goggles recommended
- No direct release to soil and surface water.

Consumer use

Because of low concentration in public used products (e.g. in fuel) the usual risk management measures when handling these (flammable) products are sufficient.
Clear spills immediately
Adult use only

State agency review

REACH-registration number 01-2119444597-28-0000

Regulatory information/classification and labelling

GHS-Labeling

Statutory basis EU-GHS as per Regulation (EU) No. 1272/2008	Pentanol, branched and linear
Symbol(s)	
Signal word	Danger
Hazard statement	H304 - May be fatal if swallowed and enters airways. H315 - Causes skin irritation.
Precautionary statements:	
Prevention	P280 – Wear protective gloves/protective clothing/eye protection/face protection.
Reaction	P302 + P352 – IF ON SKIN: Wash with plenty of soap and water. P333 + P313 – If skin irritation or rash occurs: Get medical advice/attention. P362 – Take off contaminated clothing and wash before reuse. P301 + P330 + P331 – IF SWALLOWED: rinse mouth. Do NOT induce vomiting. P310 – Immediately call a POISON CENTER or doctor/physician.

Contact information within company
Email address msds-performance-intermediates@evonik.com
Emergency Telephone number +49 (0)2365 49-2232 (Fire Brigade, Infracor GmbH)
Emergency Telefax number +49 (0)2365 49-4423

Glossary

Acute toxicity	harmful effects after a single exposure
Biodegradable	breakdown of materials by a physiological environment
Bioaccumulation	accumulation of substances in the environment
Carcinogenicity	effects causing cancer
Chronic toxicity	harmful effects after repeated exposures
GHS	Global Harmonized System on Classification and Labeling
Mutagenicity	effects that change genes
PBT	Persistent Bioaccumulative Toxic
Reprotoxicity	teratogenicity, embryotoxicity and harmful effects on fertility
Sensitizing	allergenic
Teratogenic	effects on foetal morphology
vPvB	very Persistent very Bioaccumulative

Disclaimer

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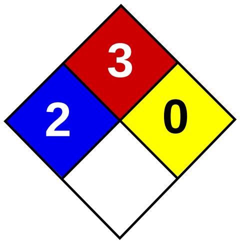
Performance of the chemical described herein should be verified by testing which should be carried out only by qualified experts.

Evonik reserves the right to make any changes to this GPS Safety Summary in accordance with technological progress or further developments. Reference to trade names used by other companies is neither a recommendation, nor does it imply, that similar products could not be used.



Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
p-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: p-Xylene

Catalog Codes: SLX1120

CAS#: 106-42-3

RTECS: ZE2625000

TSCA: TSCA 8(b) inventory: p-Xylene

CI#: Not applicable.

Synonym: p-Methyltoluene

Chemical Name: 1,4-Dimethylbenzene

Chemical Formula: $C_6H_4(CH_3)_2$

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{p-}Xylene	106-42-3	100

Toxicological Data on Ingredients: p-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 12400 mg/kg [Rabbit.]. VAPOR (LC50): Acute: 4550 ppm 4 hour(s) [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

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

Section 4: First Aid Measures

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

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

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

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

Serious Inhalation: Not available.

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

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

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

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

Flammable Limits: LOWER: 1.1% UPPER: 7%

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

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

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

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

Special Remarks on Fire Hazards:
Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

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

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

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapour/spray. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes Keep away from incompatibles such as oxidizing agents.

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

Section 8: Exposure Controls/Personal Protection

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

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

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

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

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

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

Boiling Point: 138°C (280.4°F)

Melting Point: 12°C (53.6°F)

Critical Temperature: Not available.

Specific Gravity: 0.86 (Water = 1)

Vapor Pressure: 9 mm of Hg (@ 20°C)

Vapor Density: 3.7 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.62 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

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:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 5000 mg/kg [Rat.]. Acute dermal toxicity (LD50): 12400 mg/kg [Rabbit.]. Acute toxicity of the vapor (LC50): 4550 ppm 4 hour(s) [Rat].

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

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

Special Remarks on Toxicity to Animals: Not available.

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

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

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

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

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

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Xylene : UN1307 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

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

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

Other Classifications:

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

DSCL (EEC):
R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes. R48/20- Harmful: danger of serious damage to health by prolonged exposure through inhalation.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

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

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

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

Section 16: Other Information

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

Other Special Considerations: Not available.

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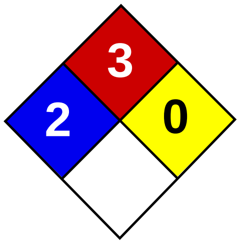

Health	2
Fire	3
Reactivity	0
Personal Protection	J

Material Safety Data Sheet

m-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: m-Xylene

Catalog Codes: SLX1066

CAS#: 108-38-3

RTECS: ZE2275000

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

CI#: Not applicable.

Synonym: m-Methyltoluene

Chemical Name: 1,3-Dimethylbenzene

Chemical Formula: C6H4(CH3)2

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{m-}Xylene	108-38-3	100

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

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

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

Section 4: First Aid Measures

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

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

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

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

Serious Inhalation: Not available.

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

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

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

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

Flammable Limits: LOWER: 1.1% UPPER: 7%

Products of Combustion: These products are carbon oxides (CO, 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 ACGIHConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

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

Boiling Point: 139.3°C (282.7°F)

Melting Point: -47.87°C (-54.2°F)

Critical Temperature: Not available.

Specific Gravity: 0.86 (Water = 1)

Vapor Pressure: 6 mm of Hg (@ 20°C)

Vapor Density: 3.7 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.62 ppm

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

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

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

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Reactive with oxidizing agents.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact.

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

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

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

Special Remarks on Toxicity to Animals: Not available.

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

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

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

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

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

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: : Xylene : UN1307 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

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

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

Other Classifications:

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

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

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: j

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

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

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

Section 16: Other Information

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

Other Special Considerations: Not available.

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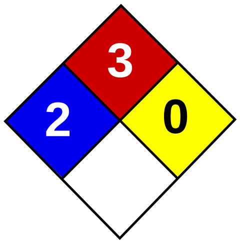

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
o-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: o-Xylene

Catalog Codes: SLX1012

CAS#: 95-47-6

RTECS: ZE2450000

TSCA: TSCA 8(b) inventory: o-Xylene

CI#: Not applicable.

Synonym: 1,2-Dimethylbenzene

Chemical Name: o-Xylene

Chemical Formula: $C_6H_4(CH_3)_2$

Contact Information:

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

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

Order Online: ScienceLab.com

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

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

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

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{o-}Xylene	95-47-6	100

Toxicological Data on Ingredients: o-Xylene LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

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

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. The substance may be toxic to kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:

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

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

Large Spill:

Toxic flammable liquid, insoluble or very slightly soluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

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

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

Section 8: Exposure Controls/Personal Protection

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

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

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

Exposure Limits:
TWA: 434 STEL: 651 (mg/m3) from ACGIH (TLV) [United States] TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) [United States] STEL: 150 (ppm) from NIOSH STEL: 655 (mg/m3) from NIOSHConsult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Mobile, nonpolar liquid.)

Odor: Aromatic. Sweetish.

Taste: Not available.

Molecular Weight: 106.17 g/mole

Color: Colorless.

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

Boiling Point: 144.4°C (291.9°F)

Melting Point: -25°C (-13°F)

Critical Temperature: 359°C (678.2°F)

Specific Gravity: 0.88 (Water = 1)

Vapor Pressure: 0.9 kPa (@ 20°C)

Vapor Density: 3.7 (Air = 1)

Volatility: Not available.

Odor Threshold: 0.05 ppm

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

Ionicity (in Water): Not available.

Dispersion Properties:
Dispersed in diethyl ether. Is not dispersed in cold water, hot water. See solubility in diethyl ether, acetone.

Solubility:
Soluble in diethyl ether, acetone. Insoluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, flames, incompatible materials.

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

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Photochemically reactive. Incompatible with strong oxidizers(e.g. chlorine, bromine, fluorine), and strong acids (e.g. nitric acid, acetic acid).

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

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

Toxicity to Animals:
Lowest Published Lethal Dose - Inhalation (LCL): 6125 ppm 12 hours [Rat]; 6125 ppm 12 hours [Human] Lowest Published Lethal Dose - Oral: 5000 mg/kg [Rat]

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. May cause damage to the following organs: kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).

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

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (male) and birth defects based on animal data. 0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Efffects Skin: May cause skin irritation. May be absorbed through skin i harmful amounts. Eyes: Causes severe eye irritation. Inhalation: Causes respiratory tract and mucous membranes irritation. May affect sense organs, behavior (Central Nervous system) which may result in dizziness, general weakness, central nervous system depression, confusion, ataxia, disorientation, lethargy, drowsiness, headaches. May also affect respiration, cardiovascular system, liver, blood, and digestive system (nausea, vomiting) Ingestion: Harmful if swallowed. Causes digestive tract irritation with nausea, vomiting

and diarrhea. May also affect metabolism, liver, and urinary system, and central nervous system (excitement followed by headache, dizziness, drowsiness and nausea). Chronic Potential Health Effects: Skin: Prolonged or repeated contact may cause defatting of skin and dermatitis. Eyes: Prolonged or repeated exposure may cause conjunctivitis or permanent eye damage. Inhalation: Chronic inhalation may cause effects similar to those of acute inhalation.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

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

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

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

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

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Xylene UNNA: 1307 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey.: o-Xylene Illinois chemical safety act: o-Xylene New York release reporting list: o-Xylene Pennsylvania RTK: o-Xylene Florida: o-Xylene Massachusetts RTK: o-Xylene Massachusetts spill list: o-Xylene New Jersey: o-Xylene New Jersey spill list: o-Xylene Louisiana spill reporting: o-Xylene California Director's List of Hazardous Substances: o-Xylene TSCA 8(b) inventory: o-Xylene TSCA 8(d) H and S data reporting: o-Xylene: Effective: 10/4/82; Sunset: 10/4/92 SARA 313 toxic chemical notification and release reporting: o-Xylene CERCLA: Hazardous substances.: o-Xylene: 1000 lbs. (453.6 kg)

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

Other Classifications:

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

DSCL (EEC):

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

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

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

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

Section 16: Other Information

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

Other Special Considerations: Not available.

Created: 10/11/2005 12:54 PM

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

MATERIAL SAFETY DATA SHEET (MSDS)
NITROGEN
(Please ensure that this MSDS is received by an appropriate person)

DATE: February 2017 Version 3 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, ¾ 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
EMERGENCY NUMBER	**0860 020202 or (011) 873 4382 (24 hours)**

2 COMPOSITION/INFORMATION ON INGREDIENTS

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

3 HAZARDS IDENTIFICATION

Main Hazards

All cylinders are portable gas containers, and must be regarded as pressure vessels at all times. Nitrogen does not support life. It can act as a simple asphyxiant by diluting the concentration of oxygen in air below the levels necessary to support life.

Adverse Health Effects

Inhalation of nitrogen in excessive concentrations can result in dizziness, nausea, vomiting, loss of consciousness and death.

Chemical Hazards

Nitrogen is relatively inert to most materials under ordinary conditions. It becomes more reactive at elevated temperatures, and combines with hydrogen, oxygen and some metals.

Biological Hazards No known effect.

Vapour Inhalation

As nitrogen acts as a simple asphyxiant death may result from errors in judgement, confusion, or loss of consciousness which prevents self-rescue. At low oxygen concentrations, unconsciousness and death may occur in seconds without warning.

4 FIRST AID MEASURES

Eye/Skin Contact	No known effect.
Ingestion	(See Section 3 above)

Inhalation

Prompt medical attention is mandatory in all cases of overexposure to Nitrogen. Rescue personnel should be equipped with self-contained breathing apparatus. Conscious persons should be assisted to an uncontaminated area and inhale fresh air. Quick removal from the contaminated area is most important. Unconscious persons should be removed to an uncontaminated area, and given mouth-to-mouth resuscitation and supplemental oxygen.

5 FIRE FIGHTING MEASURES

Extinguishing Media

As Nitrogen is an inert gas, it does not contribute to a fire, but could help with the extinguishing by reducing the oxygen content of the air by dilution to below the level to support combustion.

Specific Hazards

Nitrogen does not support life. It can act as a simple asphyxiant by diluting the concentration of oxygen in the air below the levels to support life.

Emergency Actions

If possible, shut off the source of excess Nitrogen. Evacuate area. All cylinders should be removed from the vicinity of the fire. Cylinders that cannot be removed should be cooled with water from a safe distance. Cylinders which have been exposed to excessive heat should be clearly identified and returned to supplier. CONTACT THE NEAREST AFROX BRANCH.

Protective Clothing

Self-contained breathing apparatus. Safety gloves and shoes, or boots, should be worn when handling cylinders.

Environmental Precautions

Nitrogen is lighter than air and disperses rapidly in the atmosphere. Care should be taken when entering a potentially oxygen-deficient environment. If possible, ventilate the affected area.

6 ACCIDENTAL RELEASE MEASURES

Personal Precautions

Do not enter any area where nitrogen has been spilled unless tests have shown that it is safe to do so.

Environmental Precautions

Nitrogen does not pose a hazard to the environment.

Small Spills

Shut off the source of escaping nitrogen. Ventilate the area.

Large Spills

Evacuate the area. Shut off the source of the spill if this can be done without risk. Restrict access to the area until completion of the clean-up procedure. Ventilate the area using forced-draught if necessary.

7 HANDLING AND STORAGE

Do not allow cylinders to slide or come into contact with sharp edges. Nitrogen cylinders may be stacked horizontally provided that they are firmly secured at each end to prevent rolling. Use a "first in - first out" inventory system to prevent full cylinders from being stored for excessive periods of time. Keep out of reach of children.

8 EXPOSURE CONTROLS/PERSONAL PROTECTION

Occupational Exposure Hazards

As nitrogen is a simple asphyxiant, avoid any areas where spillage has taken place. Only enter once testing has proved the atmosphere to be safe.

Engineering Control Measures

Engineering control measures are preferred to reduce exposure to Oxygen-depleted atmospheres. General methods include forced-draught ventilation, separate from other exhaust ventilation systems. Ensure that sufficient fresh air enters at, or near floor level.

Personal Protection

Self-contained breathing apparatus should always be worn when entering area where oxygen depletion may have occurred. Safety goggles, gloves and shoes or boots should be worn when handling cylinders.

Skin No known effect.

9 PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL DATA

Chemical Symbol	N_2
Molecular Weight	28,013
Specific Volume @ 20°C & 101,325 kPa	861,5ml/g
Density, gas @ 101,325 kPa and 20°C	1,25 kg/m^3
Relative density (Air = 1) @ 101,325 kPa	0,967
Colour	None
Taste	Non

MATERIAL SAFETY DATA SHEET (MSDS)

NITROGEN

(Please ensure that this MSDS is received by an appropriate person)

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

Refer to SANS 10234 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 (MSDS)
OXYGEN

(Please ensure that this MSDS is received by the appropriate person)

DATE: March 2017 Version: 4 Ref. No.: MS027

1 PRODUCT AND COMPANY IDENTIFICATION

Product Name	OXYGEN
Chemical Formula	O_2
Trade Names	Oxygen, Compressed Oxygen, Instrument Grade (N2.5) Oxygen, EP Grade (N2.7) Oxygen, IG Zero (N4.5) Oxygen, UHP (N4.5) Medical Oxygen Oxygen Agrigas Oxygen Econopack Oxygen Portapak
Colour coding	Compressed, IG, EP, IG Zero & UHP cylinders all have black bodies. Relevant decals or stencilling depict actual grades. Medical Oxygen Black Body with a white shoulder Oxygen AgriGas Black body with an orange valve guard Oxygen Econopack Black body with a blue valve guard
Valve	Compressed, IG, EP, IG Zero & Medical grades have 3 SO- Brass, 5/8 inch BSP right hand female valves. Medical oxygen cylinders could also have the revenant Pin Index valves fitted. UHP grade has the Neriki-Brass 5/8 inch BSP right hand female valve fitted.
Company Identification	African Oxygen Limited 23 Webber Street Johannesburg, 2001 Tel No: (011) 490-0400 Fax No: (011) 490-0506
EMERGENCY NUMBER	**0860 020202 or (011) 873 4382** **(24 hours)**

2 COMPOSITION/INFORMATION ON INGREDIENTS

Chemical Name	Oxygen
Chemical Family	Oxidant
CAS No	7782-44-7
UN No	1072
ERG No	122
Hazchem Warning	5 A Non-flammable Gas

3 HAZARDS IDENTIFICATION

Main Hazards

All cylinders are transportable gas containers. Oxygen is non-flammable, but readily supports combustion. Never permit oil, grease or other readily combustible substance to come into contact with high concentrations of Oxygen.

Adverse Health Effects

Central nervous system toxicity including dizziness, convulsions and loss of consciousness can occur after only 2-3 hours of exposure to pure oxygen at 2 or more atmospheres. Retrosternal soreness, associated with coughing and breathing difficulties, made worse by smoking and exposure to cold air can occur after breathing pure oxygen at atmospheric pressure for several hours.

Chemical Hazards

Oxygen is non-flammable, but strongly supports combustion (including some materials which do not normally burn in air). Since dry Oxygen is non-corrosive, most materials of construction are suitable. Avoid all flammable materials.

Biological Hazards

No known effect.

Vapour Inhalation

Pure oxygen is a local irritant to mucous membranes and, with extended continued exposure, can be destructive to lung tissue.

Label Elements

Hazard Pictograms

Signal Word: Danger

Precautionary Statements:

P220: Keep/Store away from clothing/…./ combustible materials (manufacturer/supplier or the competent authority to specify applicable ignition sources).
P244: Keep reduction valves free from grease and oil.
P370+P376: In case of fire: stop leak if safe to do so.
P403: Store in well ventilated place.

Hazard Statements:

H270: May cause or intensify fire; oxidser.

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 Oxygen. Rescue personnel should be cognisant of extreme fire hazard associated with oxygen-rich atmospheres. Conscious persons should be assisted to an uncontaminated area and inhale fresh air. They should be kept warm and quiet. Quick removal from the contaminated area is most important. The physician should be informed that the patient has experienced hyperoxia.

5 FIRE FIGHTING MEASURES

Extinguishing Media

As Oxygen is non-flammable, but strongly supports combustion; the correct type of extinguishing should be used depending on the combustible material involved.

Specific Hazards

Oxygen vigorously accelerates combustion. Materials that would not normally burn in air could combust vigorously in atmospheres having high concentrations of Oxygen.

Emergency Actions

If possible, shut off the source of escaping Oxygen. 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

Safety goggles, gloves and safety shoes should be worn when handling cylinders.

Environmental Precautions

As the gas is heavier than air, pockets of Oxygen-enriched air could occur. These could lead to the fire spreading rapidly. If possible, ventilate the affected area.

6 ACCIDENTAL RELEASE MEASURES

Personal Precautions

Although Oxygen is not itself combustible, it supports and accelerates combustion. Clothes and other materials, not normally considered flammable, will burn fiercely in the presence of Oxygen, and can be set alight by a single spark, or even hot cigarette ash.

Environmental Precautions

Oxygen does not pose a hazard to the environment. Beware of Oxygen-enriched atmospheres coming into contact with readily combustible materials. If possible, ventilate the affected area.

Small Spills

Shut off the source of excess Oxygen. Ventilate the area.

Large Spills

Evacuate the area. Shut off the source of the spill if this can be done without risk. 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. Cylinders of Oxygen should not be stored near cylinders of acetylene or other combustible gases. Oxygen cylinders may be stacked horizontally provided that they are firmly secured at each end to prevent rolling. Prevent dirt, grit of any sort, oil or any other lubricant from entering the cylinder valves, and store cylinders well clear of any corrosive influence, e.g. battery acid. Compliance with all relevant legislation is essential. 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

Avoid exposure to oxygen-enriched atmospheres, as this could result in clothing becoming saturated by oxygen. On ignition the clothing could burn fiercely resulting in serious burns.

Engineering Control Measures

Engineering control measures are preferred to reduce exposure to Oxygen-enriched 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

Safety goggles, gloves and shoes should be worn when handling cylinders.

Skin

No known effect.

9 PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL DATA

Chemical Symbol	O_2
Molecular Weight	32,00
Specific Volume @ 20°C & 101,325 kPa	755 ml/g
Boiling Point 101,325 kPa	90.18 °K; -183 °C; 181.4 °F
Density, gas @ 101,325 kPa and 20°C	1,33 kg/m^3
Relative density (Air = 1) @ 101,325 kPa	1,053
Solubility in Water @ 101.325 kPa @ 25 °C	
(Partial Pressure of O_2) @ O °C	4.889 cm^3 O_2/100 cm^3 water
Colour	None
Taste	None
Odour	None

10 STABILITY AND REACTIVITY

Conditions to avoid

The build up of Oxygen-enriched atmospheres as, depending on temperature, oxygen reacts with all of the elements, excepting the inert gases, to form oxides. These reactions can sometimes be

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

Oxygen is heavier than air and care should be taken to avoid the formation of Oxygen-enriched pockets. It does not pose a hazard to the ecology.

13 DISPOSAL CONSIDERATIONS

Disposal Methods

Small amounts may be blown to atmosphere under controlled conditions. Large amounts should only be handled by gas supplier.

Disposal of Packaging

The disposal of containers must only be handled by the gas supplier.

14 TRANSPORT INFORMATION

ROAD TRANSPORTATION

UN No	1072
ERG No	122
Hazchem warning	5A Non-flammable Gas

SEA TRANSPORTATION

IMDG	1072
Class	
Packaging group	
Label	Non-flammable Gas

AIR TRANSPORTATION

ICAO/IATA Code	1072
Class	Non-flammable
Packaging group	2.2
Packaging instructions	
- Cargo	200
- Passenger	200
Maximum quantity allowed	
- Cargo	100kg
- Passenger	75kg

15 REGULATORY INFORMATION

EEC Hazard class Non-flammable
National legislation OHSact and Regulations 85 of 1993.
Reference SANS 10234 and its supplement.

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

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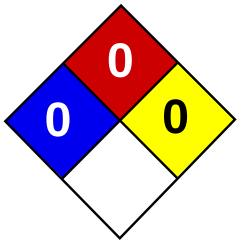


Health	0
Fire	0
Reactivity	0
Personal Protection	A

Material Safety Data Sheet

Water MSDS

Section 1: Chemical Product and Company Identification

Product Name: Water

Catalog Codes: SLW1063

CAS#: 7732-18-5

RTECS: ZC0110000

TSCA: TSCA 8(b) inventory: Water

CI#: Not available.

Synonym: Dihydrogen oxide

Chemical Name: Water

Chemical Formula: H_2O

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
Water	7732-18-5	100

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

Potential Acute Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Potential Chronic Health Effects:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-irritating to the eyes. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available.

Section 4: First Aid Measures

Eye Contact: Not applicable.

Skin Contact: Not applicable.

Serious Skin Contact: Not available.

Inhalation: Not applicable.

Serious Inhalation: Not available.

Ingestion: Not Applicable

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances: Not Applicable

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

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

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

Section 7: Handling and Storage

Precautions: No specific safety phrase has been found applicable for this product.

Storage: Not applicable.

Section 8: Exposure Controls/Personal Protection

Engineering Controls: Not Applicable

Personal Protection: Safety glasses. Lab coat.

Personal Protection in Case of a Large Spill: Not Applicable

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Odorless.

Taste: Not available.

Molecular Weight: 18.02 g/mole

Color: Colorless.

pH (1% soln/water): 7 [Neutral.]

Boiling Point: 100°C (212°F)

Melting Point: Not available.

Critical Temperature: Not available.

Specific Gravity: 1 (Water = 1)

Vapor Pressure: 2.3 kPa (@ 20°C)

Vapor Density: 0.62 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not applicable

Solubility: Not Applicable

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Not available.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact.

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

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Non-corrosive for skin. Non-irritant for skin. Non-sensitizer for skin. Non-permeator by skin. Non-hazardous in case of ingestion. Non-hazardous in case of inhalation. Non-irritant for lungs. Non-sensitizer for lungs. Non-corrosive to the eyes. Non-corrosive for lungs.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

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

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

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

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

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

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Water

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC):
This product is not classified according to the EU regulations. Not applicable.

HMIS (U.S.A.):

Health Hazard: 0

Fire Hazard: 0

Reactivity: 0

Personal Protection: a

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

Health: 0

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

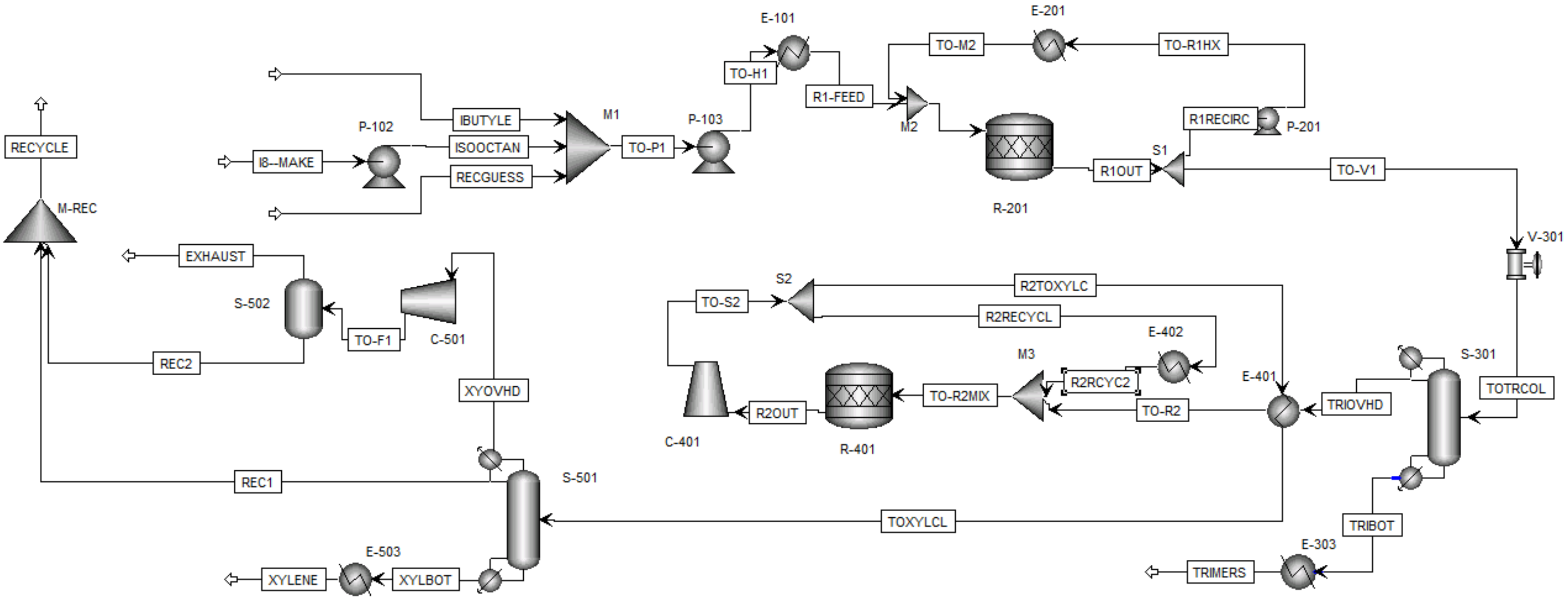
References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM

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

Section 25.5
ASPEN Reports


E-101
E-201
TO-M2
TO-R1HX
TO-H1
R1-FEED
M2
R1RECIRC
P-201
IBUTYLE
P-102
ISOOCTAN
M1
TO-P1
P-103
S1
I8--MAKE
RECGUESS
R1OUT
TO-V1
R-201
RECYCLE
M-REC
V-301
EXHAUST
S2
S-502
TO-S2
R2TOXYLC
R2RECYCL
E-402
TO-F1
C-501
S-301
REC2
M3
R2RCYC2
E-401
XYOVHD
TOTRCOL
TO-R2MIX
R2OUT
TO-R2
TRIOVHD
C-401
R-401
S-501
REC1
TOXYLCL
TRIBOT
E-503
E-303
XYLENE
XYLBOT
TRIMERS

```
;
;Input Summary created by Aspen Plus Rel. 36.0 at 22:11:13 Sun Apr 8,
2018
;Directory \\nestor\xiaoxint\March 25 (1)  Filename
C:\Users\xiaoxint\AppData\Local\Temp\~ap1466.txt
;


DYNAMICS
    DYNAMICS RESULTS=ON

IN-UNITS ENG SHORT-LENGTH=in

DEF-STREAMS CONVEN ALL

MODEL-OPTION

DATABANKS 'APV100 PURE36' / 'APV100 AQUEOUS' / 'APV100 SOLIDS' &
         / 'APV100 INORGANIC' / 'APESV100 AP-EOS' /  &
        'NISTV100 NIST-TRC' / NOASPENPCD

PROP-SOURCES 'APV100 PURE36' / 'APV100 AQUEOUS' /  &
        'APV100 SOLIDS' / 'APV100 INORGANIC' / 'APESV100 AP-EOS' &
         / 'NISTV100 NIST-TRC'

COMPONENTS
    ISOBUTYL C4H8-5 /
    ISOOCTAN C8H18-13 /
    2:4:4-01 C8H16-D4 /
    TRIMERS C12H24-2 /
    M-XYL-01 C8H10-2 /
    O-XYL-01 C8H10-1 /
    P-XYL-01 C8H10-3 /
    HYDROGEN H2

HENRY-COMPS HC-1 HYDROGEN

SOLVE
    RUN-MODE MODE=SIM

FLOWSHEET
    BLOCK M1 IN=IBUTYLE RECGUESS ISOOCTAN OUT=TO-P1
    BLOCK P-102 IN=TO-P1 OUT=TO-H1
    BLOCK E-101 IN=TO-H1 OUT=R1-FEED
    BLOCK R-201 IN=TO-R1 OUT=R1OUT
    BLOCK R-401 IN=TO-R2MIX OUT=R2OUT
    BLOCK E-401 IN=R2TOXYLC TRIOVHD OUT=TOXYLCL TO-R2
    BLOCK S-501 IN=TOXYLCL OUT=XYOVHD REC1 XYLBOT
    BLOCK S-301 IN=TOTRCOL OUT=TRIOVHD TRIBOT
    BLOCK M2 IN=R1-FEED TO-M2 OUT=TO-R1
    BLOCK S1 IN=R1OUT OUT=R1RECIRC TO-V1
    BLOCK E-201 IN=TO-R1HX OUT=TO-M2
    BLOCK P-201 IN=R1RECIRC OUT=TO-R1HX
    BLOCK S2 IN=TO-S2 OUT=R2TOXYLC R2RECYCL
    BLOCK E-402 IN=R2RECYCL OUT=R2RCYC2
    BLOCK C-401 IN=R2OUT OUT=TO-S2
    BLOCK M3 IN=TO-R2 R2RCYC2 OUT=TO-R2MIX
    BLOCK C-501 IN=XYOVHD OUT=TO-F1
    BLOCK S-502 IN=TO-F1 OUT=EXHAUST REC2
    BLOCK M-REC IN=REC1 REC2 OUT=RECYCLE
```

```
    BLOCK E-503 IN=XYLBOT OUT=XYLENE
    BLOCK E-303 IN=TRIBOT OUT=TRIMERS
    BLOCK V-301 IN=TO-V1 OUT=TOTRCOL
    BLOCK P-101 IN=I8--MAKE OUT=ISOOCTAN

PROPERTIES NRTL

PROP-DATA HENRY-1
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar' SHORT-LENGTH=mm
    PROP-LIST HENRY
    BPVAL HYDROGEN ISOOCTAN 17.48877354 -43.41299800  &
        -1.786100000 0.0 -25.00000000 35.00000000 0.0
    BPVAL HYDROGEN M-XYL-01 5.774775535 604.1699830 0.0 0.0  &
        18.00000000 32.10000000 0.0

PROP-DATA NRTL-1
    IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
        INVERSE-PRES='1/bar' SHORT-LENGTH=mm
    PROP-LIST NRTL
    BPVAL M-XYL-01 O-XYL-01 0.0 -248.9737000 .3000000000 0.0  &
        0.0 0.0 65.00000000 85.00000000
    BPVAL O-XYL-01 M-XYL-01 0.0 337.2790000 .3000000000 0.0  &
        0.0 0.0 65.00000000 85.00000000
    BPVAL M-XYL-01 P-XYL-01 0.0 4.630100000 .3000000000 0.0  &
        0.0 0.0 138.3500000 139.1000000
    BPVAL P-XYL-01 M-XYL-01 0.0 -3.869000000 .3000000000 0.0  &
        0.0 0.0 138.3500000 139.1000000

STREAM I8--MAKE
    SUBSTREAM MIXED TEMP=80. PRES=15.
    MASS-FLOW ISOOCTAN 445.37

STREAM IBUTYLE
    SUBSTREAM MIXED TEMP=10. PRES=20.
    MASS-FLOW ISOBUTYL 126820.

STREAM RECGUESS
    SUBSTREAM MIXED TEMP=86. PRES=29.3959
    MASS-FLOW ISOBUTYL 1070.2877965 / ISOOCTAN 42948.577056 /  &
        2:4:4-01 9920.8508263 / TRIMERS 0.00034124198 /  &
        M-XYL-01 36.180805614 / O-XYL-01 13.934467023 /  &
        P-XYL-01 742.82855661 / HYDROGEN 0.45554575933

BLOCK M-REC MIXER
    PARAM

BLOCK M1 MIXER
    PARAM

BLOCK M2 MIXER
    PARAM

BLOCK M3 MIXER
    PARAM

BLOCK S1 FSPLIT
    MASS-FLOW R1RECIRC 895140.

BLOCK S2 FSPLIT
```

```
    MASS-FLOW R2RECYCL 1470000.

BLOCK E-101 HEATER
    PARAM TEMP=347.0000000 PRES=764.6959488 DPPARMOPT=NO

BLOCK E-201 HEATER
    PARAM TEMP=300. PRES=0. DPPARMOPT=NO

BLOCK E-303 HEATER
    PARAM TEMP=80. PRES=60. DPPARMOPT=NO

BLOCK E-402 HEATER
    PARAM TEMP=1050. PRES=0. DPPARMOPT=NO

BLOCK E-503 HEATER
    PARAM TEMP=80. PRES=35. DPPARMOPT=NO

BLOCK S-502 FLASH2
    PARAM TEMP=40. PRES=0.

BLOCK E-401 HEATX
    PARAM DELT-HOT=50. CALC-TYPE=DESIGN PRES-HOT=45.  &
        U-OPTION=PHASE F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
    FEEDS HOT=R2TOXYLC COLD=TRIOVHD
    OUTLETS-HOT TOXYLCL
    OUTLETS-COLD TO-R2
    HOT-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    COLD-SIDE DP-OPTION=CONSTANT DPPARMOPT=NO
    TQ-PARAM CURVE=YES

BLOCK S-301 RADFRAC
    SUBOBJECTS INTERNALS = CS-1
    PARAM NSTAGE=9 ALGORITHM=STANDARD MAXOL=100 DAMPING=NONE
    PARAM2 STATIC-DP=YES
    COL-CONFIG CONDENSER=TOTAL CA-CONFIG=INT-1
    FEEDS TOTRCOL 6 ON-STAGE
    PRODUCTS TRIBOT 9 L / TRIOVHD 1 L
    P-SPEC 1 70.
    COL-SPECS DP-STAGE=0.12 MOLE-B=230.1 MOLE-RR=4.  &
        DP-COND=2.000000000
    SPEC 1 MOLE-RECOV 0.98 COMPS=TRIMERS STREAMS=TRIBOT  &
        SPEC-DESCRIP="Mole recovery, 0.98"
    SPEC 2 MASS-FRAC 0.98 COMPS=TRIMERS STREAMS=TRIBOT  &
        SPEC-DESCRIP="Mass purity, 0.98, PRODUCT"
    VARY 1 MOLE-B 153.6 384.
    VARY 2 MOLE-RR 0. 10.
    INTERNALS CS-1 STAGE1=2 STAGE2=8 P-UPDATE=NO TRAY-SPACE=1.5
    TRAY-SIZE 1 2 8 SIEVE

BLOCK S-501 RADFRAC
    SUBOBJECTS INTERNALS = CS-1
    PARAM NSTAGE=16 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=80  &
        DAMPING=NONE
    PARAM2 STATIC-DP=YES
    COL-CONFIG CONDENSER=PARTIAL-V-L CA-CONFIG=INT-1
    FEEDS TOXYLCL 5 ON-STAGE
    PRODUCTS XYLBOT 16 L / REC1 1 L / XYOVHD 1 V
    P-SPEC 1 39.
    COL-SPECS DP-STAGE=0.12 MASS-B=75000. MASS-RR=6. DP-COND=4.  &
        T1=100.
```

```
    SPEC 1 MASS-RECOV 0.99 COMPS=M-XYL-01 O-XYL-01 P-XYL-01  &
        STREAMS=XYLBOT SPEC-ACTIVE=YES  &
        SPEC-DESCRIP="Mass recovery"
    SPEC 2 MASS-RECOV 0.99 COMPS=M-XYL-01 O-XYL-01 P-XYL-01  &
        STREAMS=XYLBOT SPEC-ACTIVE=YES  &
        SPEC-DESCRIP="Mass recovery, 0.99"
    VARY 1 MASS-B 25590. 110000. VARY-ACTIVE=YES
    VARY 2 MASS-RR 0.7 20. VARY-ACTIVE=YES
    REPORT NOHYDRAULIC
    INTERNALS CS-1 STAGE1=2 STAGE2=15 P-UPDATE=NO NPASS=1
    TRAY-SIZE 1 2 15 SIEVE

BLOCK R-201 RSTOIC
    PARAM PRES=764.6959488 DUTY=0. HEAT-OF-REAC=YES
    STOIC 1 MIXED ISOBUTYL -2. / 2:4:4-01 1.
    STOIC 2 MIXED ISOBUTYL -3. / TRIMERS 1.
    CONV 1 MIXED ISOBUTYL 0.6
    CONV 2 MIXED ISOBUTYL 0.3
    HEAT-RXN REACNO=1 CID=ISOBUTYL PHASE=L / REACNO=2  &
        CID=ISOBUTYL PHASE=L

BLOCK R-401 RSTOIC
    PARAM PRES=36.69594878 DUTY=0.
    STOIC 1 MIXED 2:4:4-01 -1. / P-XYL-01 1. / HYDROGEN 3.
    STOIC 2 MIXED 2:4:4-01 -1. / O-XYL-01 1. / HYDROGEN 3.
    STOIC 3 MIXED 2:4:4-01 -1. / M-XYL-01 1. / HYDROGEN 3.
    CONV 1 MIXED 2:4:4-01 0.378
    CONV 2 MIXED 2:4:4-01 0.021
    CONV 3 MIXED 2:4:4-01 0.021

BLOCK P-101 PUMP
    PARAM DELP=20. <psia>

BLOCK P-102 PUMP
    PARAM PRES=764.6959488

BLOCK P-201 PUMP
    PARAM DELP=20. EFF=0.8

BLOCK C-401 COMPR
    PARAM TYPE=ISENTROPIC PRES=45. SEFF=0.85 SB-MAXIT=30  &
        SB-TOL=0.0001

BLOCK C-501 COMPR
    PARAM TYPE=ISENTROPIC PRES=300. SEFF=0.85 SB-MAXIT=30  &
        SB-TOL=0.0001

BLOCK V-301 VALVE
    PARAM P-OUT=80.

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW

PROP-TABLE PURE-1 PROPS
    IN-UNITS ENG PRESSURE=bar TEMPERATURE=C PDROP=psi  &
        SHORT-LENGTH=in
    ANALYSIS ANAL-TYPE=PURE PURE-PROP='AVAIL' PURE-PHASES= L
    MOLE-FLOW TRIMERS 1
    PROPERTIES NRTL FREE-WATER=STEAM-TA SOLU-WATER=3  &
```

```
        TRUE-COMPS=YES
    VARY TEMP
    RANGE VARVALUE=RANGE LOWER=0 UPPER=100.0000000 NPOINT=50
    VARY PRES
    RANGE LIST=1.013250000
    PARAM
;
;
;
;
;
```

```
 BLOCK:  C-401    MODEL: COMPR
 ----------------------------
   INLET STREAM:          R2OUT
   OUTLET STREAM:         TO-S2
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           40000.7        40000.7         0.00000
       MASS(LB/HR   )         0.161015E+07    0.161015E+07     0.00000
       ENTHALPY(BTU/HR  )     0.545006E+09    0.573019E+09   -
0.488854E-01

                     ***  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 CENTRIFUGAL COMPRESSOR
    OUTLET PRESSURE  PSIA                                  45.0000
    ISENTROPIC EFFICIENCY                                   0.85000
    MECHANICAL EFFICIENCY                                   1.00000

                          ***  RESULTS  ***

    INDICATED  HORSEPOWER REQUIREMENT  HP              11,009.2
    BRAKE      HORSEPOWER REQUIREMENT  HP              11,009.2
    NET WORK REQUIRED                  HP              11,009.2
    POWER LOSSES                       HP                   0.0
    ISENTROPIC HORSEPOWER REQUIREMENT  HP               9,357.85
    CALCULATED OUTLET TEMP  F                           1,022.11
    ISENTROPIC TEMPERATURE  F                           1,018.88
    EFFICIENCY (POLYTR/ISENTR) USED                         0.85000
    OUTLET VAPOR FRACTION                                   1.00000
    HEAD DEVELOPED,       FT-LBF/LB                    11,507.3
    MECHANICAL EFFICIENCY USED                              1.00000
    INLET HEAT CAPACITY RATIO                               1.06545
    INLET VOLUMETRIC FLOW RATE , CUFT/HR                    0.170814+08
    OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                    0.141350+08
    INLET  COMPRESSIBILITY FACTOR                           1.00000
    OUTLET COMPRESSIBILITY FACTOR                           1.00000
    AV. ISENT. VOL. EXPONENT                                1.06516
    AV. ISENT. TEMP EXPONENT                                1.06516
    AV. ACTUAL VOL. EXPONENT                                1.07742
    AV. ACTUAL TEMP EXPONENT                                1.07742

 BLOCK:  C-501    MODEL: COMPR
 ----------------------------
   INLET STREAM:          XYOVHD
   OUTLET STREAM:         TO-F1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                     ***  MASS AND ENERGY BALANCE  ***
```

```
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            2357.93         2357.93         0.00000
       MASS(LB/HR   )            17901.6         17901.6
0.203220E-15
       ENTHALPY(BTU/HR  )      -0.844451E+07    -536402.       -0.936479

                      ***  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 CENTRIFUGAL COMPRESSOR
    OUTLET PRESSURE  PSIA                                   300.000
    ISENTROPIC EFFICIENCY                                     0.85000
    MECHANICAL EFFICIENCY                                     1.00000

                           ***  RESULTS  ***

    INDICATED  HORSEPOWER REQUIREMENT  HP                 3,108.00
    BRAKE      HORSEPOWER REQUIREMENT  HP                 3,108.00
    NET WORK REQUIRED                  HP                 3,108.00
    POWER LOSSES                       HP                     0.0
    ISENTROPIC HORSEPOWER REQUIREMENT  HP                 2,641.80
    CALCULATED OUTLET TEMP  F                               454.070
    ISENTROPIC TEMPERATURE  F                               403.667
    EFFICIENCY (POLYTR/ISENTR) USED                           0.85000
    OUTLET VAPOR FRACTION                                     1.00000
    HEAD DEVELOPED,       FT-LBF/LB                     292,195.
    MECHANICAL EFFICIENCY USED                                1.00000
    INLET HEAT CAPACITY RATIO                                 1.29251
    INLET VOLUMETRIC FLOW RATE , CUFT/HR                363,123.
    OUTLET VOLUMETRIC FLOW RATE, CUFT/HR                 77,070.5
    INLET  COMPRESSIBILITY FACTOR                             1.00000
    OUTLET COMPRESSIBILITY FACTOR                             1.00000
    AV. ISENT. VOL. EXPONENT                                  1.26977
    AV. ISENT. TEMP EXPONENT                                  1.26977
    AV. ACTUAL VOL. EXPONENT                                  1.31625
    AV. ACTUAL TEMP EXPONENT                                  1.31625

 BLOCK:  E-101    MODEL: HEATER
 ------------------------------
   INLET STREAM:          TO-H1
   OUTLET STREAM:         R1-FEED
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            2755.36         2755.36         0.00000
       MASS(LB/HR   )            181998.         181998.         0.00000
       ENTHALPY(BTU/HR  )      -0.885408E+08   -0.403164E+08   -0.544657

                      ***  CO2 EQUIVALENT SUMMARY ***
```

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

                          ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE                F                       347.000
   SPECIFIED PRESSURE                   PSIA                    764.696
   MAXIMUM NO. ITERATIONS                                        30
   CONVERGENCE TOLERANCE
0.000100000



                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    347.00
   OUTLET PRESSURE       PSIA                                 764.70
   HEAT DUTY             BTU/HR                              0.48224E+08
   OUTLET VAPOR FRACTION                                     0.81361E-01



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      ISOBUTYL         0.82725        0.81381        0.97906
1.2031
      ISOOCTAN         0.13787        0.14863        0.16313E-01
0.10975
      2:4:4-01         0.32086E-01    0.34616E-01    0.35260E-02
0.10186
      TRIMERS          0.73577E-09    0.80044E-09    0.56165E-11
0.70168E-02
      M-XYL-01         0.12368E-03    0.13409E-03    0.61799E-05
0.46088E-01
      O-XYL-01         0.47634E-04    0.51667E-04    0.20984E-05
0.40614E-01
      P-XYL-01         0.25393E-02    0.27528E-02    0.12849E-03
0.46676E-01
      HYDROGEN         0.82014E-04    0.35383E-05    0.96808E-03
273.60

 BLOCK:  E-201    MODEL: HEATER
 ------------------------------
   INLET STREAM:          TO-R1HX
   OUTLET STREAM:         TO-M2
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           7438.37         7438.36
0.104693E-05
       MASS(LB/HR   )           895140.         895141.        -
0.118949E-05
       ENTHALPY(BTU/HR  )     -0.423402E+09   -0.469316E+09
0.978325E-01
```

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

                       ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE               F                       300.000
   PRESSURE DROP                       PSI                       0.0
   MAXIMUM NO. ITERATIONS                                       30
   CONVERGENCE TOLERANCE
0.000100000



                        ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    300.00
   OUTLET PRESSURE       PSIA                                 784.70
   HEAT DUTY             BTU/HR                             -0.45923E+08
   OUTLET VAPOR FRACTION                                      0.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)          X(I)          Y(I)          K(I)
      ISOBUTYL        0.27774E-01   0.27774E-01   0.19792
0.79119
      ISOOCTAN        0.25109       0.25109       0.14367
0.63528E-01
      2:4:4-01        0.55164       0.55164       0.29405
0.59184E-01
      TRIMERS         0.16440       0.16440       0.44311E-02
0.29925E-02
      M-XYL-01        0.22538E-03   0.22538E-03   0.49087E-04
0.24182E-01
      O-XYL-01        0.86802E-04   0.86802E-04   0.16509E-04
0.21117E-01
      P-XYL-01        0.46277E-02   0.46277E-02   0.10257E-02
0.24609E-01
      HYDROGEN        0.14943E-03   0.14943E-03   0.35884
266.63

 BLOCK:  E-303    MODEL: HEATER
 ------------------------------
   INLET STREAM:          TRIBOT
   OUTLET STREAM:         TRIMERS
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                   ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)          251.124         251.124         0.00000
       MASS(LB/HR   )          41851.7         41851.7         0.00000
       ENTHALPY(BTU/HR  )    -0.116336E+08   -0.239254E+08    0.513755
```

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

                            ***  INPUT DATA  ***
        TWO    PHASE  TP  FLASH
        SPECIFIED TEMPERATURE                F                         80.0000
        SPECIFIED PRESSURE                   PSIA                      60.0000
        MAXIMUM NO. ITERATIONS                                         30
        CONVERGENCE TOLERANCE
     0.000100000



                             ***  RESULTS  ***
        OUTLET TEMPERATURE    F                                     80.000
        OUTLET PRESSURE       PSIA                                  60.000
        HEAT DUTY             BTU/HR                              -0.12292E+08
        OUTLET VAPOR FRACTION                                       0.0000



        V-L PHASE EQUILIBRIUM :

           COMP              F(I)           X(I)           Y(I)           K(I)
           ISOBUTYL         0.14314E-06    0.14314E-06    0.21549E-03
     0.77123
           ISOOCTAN         0.73024E-02    0.73024E-02    0.24535
     0.17212E-01
           2:4:4-01         0.20140E-01    0.20140E-01    0.61337
     0.15601E-01
           TRIMERS          0.97031        0.97031        0.12751
     0.67317E-04
           M-XYL-01         0.10383E-03    0.10383E-03    0.60385E-03
     0.29792E-02
           O-XYL-01         0.59598E-04    0.59598E-04    0.27488E-03
     0.23627E-02
           P-XYL-01         0.20873E-02    0.20873E-02    0.12677E-01
     0.31114E-02

      BLOCK:  E-401    MODEL: HEATX
      -----------------------------
        HOT SIDE:
        ---------
        INLET STREAM:             R2TOXYLC
        OUTLET STREAM:            TOXYLCL
        PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS
        COLD SIDE:
        ----------
        INLET STREAM:             TRIOVHD
        OUTLET STREAM:            TO-R2
        PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

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

```
       MOLE(LBMOL/HR)            4742.93         4742.93         0.00000
       MASS(LB/HR   )            280296.         280296.         0.00000
       ENTHALPY(BTU/HR  )      -0.324614E+08   -0.324614E+08   -
0.573804E-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  ***

   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                         50.0000
     TEMPERATURE TOLERANCE        F                          0.01800
     LMTD CORRECTION FACTOR                                  1.00000

   PRESSURE SPECIFICATION:
     HOT  SIDE OUTLET PRESSURE    PSIA                      45.0000
     COLD SIDE PRESSURE DROP      PSI                        0.0000

   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:
                   --------------------------------------
                   |                                    |
   R2TOXYLC  ----->|               HOT                  |-----> TOXYLCL
   T=  1.0221D+03  |                                    |       T=
2.8957D+02
   P=  4.5000D+01  |                                    |       P=
4.5000D+01
   V=  1.0000D+00  |                                    |       V=
1.0000D+00
                   |                                    |
   TO-R2     <-----|               COLD                 |<----- TRIOVHD
```

```
   T=  8.5577D+02  |                                     |       T=
2.3957D+02
   P=  7.0000D+01  |                                     |       P=
7.0000D+01
   V=  1.0000D+00  |                                     |       V=
0.0000D+00
                   --------------------------------------

   DUTY AND AREA:
     CALCULATED HEAT DUTY           BTU/HR            70869597.8555
     CALCULATED (REQUIRED) AREA     SQFT                  2984.6896
     ACTUAL EXCHANGER AREA          SQFT                  2984.6896
     PER CENT OVER-DESIGN                                    0.0000

   HEAT TRANSFER COEFFICIENT:
     AVERAGE COEFFICIENT (DIRTY)    BTU/HR-SQFT-R          149.6937
     UA (DIRTY)                     BTU/HR-R            446789.0937

   LOG-MEAN TEMPERATURE DIFFERENCE:
     LMTD CORRECTION FACTOR                                  1.0000
     LMTD (CORRECTED)               F                      158.6198
     NUMBER OF SHELLS IN SERIES                                1

   PRESSURE DROP:
     HOTSIDE, TOTAL                 PSI                      0.0000
     COLDSIDE, TOTAL                PSI                      0.0000

                        ***  ZONE RESULTS  ***

   TEMPERATURE LEAVING EACH ZONE:

                                     HOT
         -------------------------------------------------------------
         |                             |                             |
 HOT IN  |             VAP             |             VAP             |
HOT OUT
 ------> |                             |                             |---
--->
 1022.1  |                        560.5|                             |
289.6
         |                             |                             |
 COLDOUT |             VAP             |             BOIL            |
COLDIN
 <------ |                             |                             |<--
----
  855.8  |                        337.8|                             |
239.6
         |                             |                             |
         -------------------------------------------------------------
                                     COLD

   ZONE HEAT TRANSFER AND AREA:

   ZONE       HEAT DUTY       AREA        LMTD        AVERAGE U       UA
              BTU/HR          SQFT         F          BTU/HR-SQFT-R
BTU/HR-R
     1   47865700.936      1655.4764     193.1515   149.6937
247814.3115
     2   23003896.920      1329.2132     115.6121   149.6937
198974.7823
```

```
HEATX COLD-TQCU E-401    TQCURV INLET
-------------------------------------
  PRESSURE PROFILE:      CONSTANT2
  PRESSURE DROP:         0.0         PSI
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

-----------------------------------------------------
!  DUTY      !  PRES      !  TEMP      !  VFRAC     !
!            !            !            !            !
!            !            !            !            !
!            !            !            !            !
!  BTU/HR    !  PSIA      !  F         !            !
!            !            !            !            !
!============!============!============!============!
!     0.0    !    70.0000 !   855.7711 !     1.0000 !
!  3.3747+06 !    70.0000 !   823.8618 !     1.0000 !
!  6.7495+06 !    70.0000 !   791.4802 !     1.0000 !
!  1.0124+07 !    70.0000 !   758.5912 !     1.0000 !
!  1.3499+07 !    70.0000 !   725.1554 !     1.0000 !
!------------+------------+------------+------------!
!  1.6874+07 !    70.0000 !   691.1282 !     1.0000 !
!  2.0248+07 !    70.0000 !   656.4583 !     1.0000 !
!  2.3623+07 !    70.0000 !   621.0867 !     1.0000 !
!  2.6998+07 !    70.0000 !   584.9447 !     1.0000 !
!  3.0373+07 !    70.0000 !   547.9512 !     1.0000 !
!------------+------------+------------+------------!
!  3.3747+07 !    70.0000 !   510.0096 !     1.0000 !
!  3.7122+07 !    70.0000 !   471.0030 !     1.0000 !
!  4.0497+07 !    70.0000 !   430.7881 !     1.0000 !
!  4.3872+07 !    70.0000 !   389.1858 !     1.0000 !
!  4.7246+07 !    70.0000 !   345.9692 !     1.0000 !
!------------+------------+------------+------------!
!  4.7866+07 !    70.0000 !   337.8412 ! DEW>1.0000 !
!  5.0621+07 !    70.0000 !   333.3303 !     0.8298 !
!  5.3996+07 !    70.0000 !   331.2547 !     0.6006 !
!  5.7371+07 !    70.0000 !   328.6265 !     0.3751 !
!  6.0745+07 !    70.0000 !   322.9392 !     0.1685 !
!------------+------------+------------+------------!
!  6.4120+07 !    70.0000 !   307.7922 !  1.8232-02 !
!  6.7495+07 !    70.0000 !   275.7111 !  3.0604-04 !
!  7.0870+07 !    70.0000 !   239.5669 !  5.7269-08 !
-----------------------------------------------------

HEATX HOT-TQCUR E-401    TQCURV INLET
-------------------------------------
  PRESSURE PROFILE:      CONSTANT2
  PRESSURE DROP:         0.0         PSI
  PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

-----------------------------------------------------
!  DUTY      !  PRES      !  TEMP      !  VFRAC     !
!            !            !            !            !
!            !            !            !            !
!            !            !            !            !
!  BTU/HR    !  PSIA      !  F         !            !
!            !            !            !            !
!============!============!============!============!
!     0.0    !    45.0000 !  1022.1082 !     1.0000 !
!  3.3747+06 !    45.0000 !   992.2229 !     1.0000 !
```

```
 !  6.7495+06 !    45.0000 !   962.0273 !     1.0000 !
 !  1.0124+07 !    45.0000 !   931.5043 !     1.0000 !
 !  1.3499+07 !    45.0000 !   900.6352 !     1.0000 !
 !------------+------------+------------+------------!
 !  1.6874+07 !    45.0000 !   869.3995 !     1.0000 !
 !  2.0248+07 !    45.0000 !   837.7750 !     1.0000 !
 !  2.3623+07 !    45.0000 !   805.7374 !     1.0000 !
 !  2.6998+07 !    45.0000 !   773.2597 !     1.0000 !
 !  3.0373+07 !    45.0000 !   740.3122 !     1.0000 !
 !------------+------------+------------+------------!
 !  3.3747+07 !    45.0000 !   706.8617 !     1.0000 !
 !  3.7122+07 !    45.0000 !   672.8711 !     1.0000 !
 !  4.0497+07 !    45.0000 !   638.2985 !     1.0000 !
 !  4.3872+07 !    45.0000 !   603.0962 !     1.0000 !
 !  4.7246+07 !    45.0000 !   567.2095 !     1.0000 !
 !------------+------------+------------+------------!
 !  4.7866+07 !    45.0000 !   560.5447 !     1.0000 !
 !  5.0621+07 !    45.0000 !   530.5746 !     1.0000 !
 !  5.3996+07 !    45.0000 !   493.1170 !     1.0000 !
 !  5.7371+07 !    45.0000 !   454.7473 !     1.0000 !
 !  6.0745+07 !    45.0000 !   415.3579 !     1.0000 !
 !------------+------------+------------+------------!
 !  6.4120+07 !    45.0000 !   374.8163 !     1.0000 !
 !  6.7495+07 !    45.0000 !   332.9565 !     1.0000 !
 !  7.0870+07 !    45.0000 !   289.5669 !     1.0000 !
 -----------------------------------------------------

 BLOCK:  E-402    MODEL: HEATER
 ------------------------------
   INLET STREAM:          R2RECYCL
   OUTLET STREAM:         R2RCYC2
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            36519.0         36519.0         0.00000
       MASS(LB/HR   )         0.147000E+07    0.147000E+07     0.00000
       ENTHALPY(BTU/HR  )     0.523143E+09    0.556498E+09   -
0.599379E-01

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

                          ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE                F                     1,050.00
   PRESSURE DROP                        PSI                       0.0
   MAXIMUM NO. ITERATIONS                                        30
   CONVERGENCE TOLERANCE
0.000100000


                           ***  RESULTS  ***
```

```
   OUTLET TEMPERATURE    F                                    1050.0
   OUTLET PRESSURE       PSIA                                 45.000
   HEAT DUTY             BTU/HR                              0.33355E+08
   OUTLET VAPOR FRACTION                                      1.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      ISOBUTYL         0.12070E-01    0.72368E-02    0.12070E-01
394.47
      ISOOCTAN         0.10858        0.25575        0.10858
100.41
      2:4:4-01         0.25554E-01    0.46505E-01    0.25554E-01
129.96
      TRIMERS          0.14295E-02    0.86438E-02    0.14295E-02
39.114
      M-XYL-01         0.10718E-01    0.32548E-01    0.10718E-01
77.888
      O-XYL-01         0.10659E-01    0.34294E-01    0.10659E-01
73.508
      P-XYL-01         0.19318        0.58258        0.19318
78.428
      HYDROGEN         0.63781        0.32447E-01    0.63781
4649.1

 BLOCK:  E-503    MODEL: HEATER
 ------------------------------
   INLET STREAM:          XYLBOT
   OUTLET STREAM:         XYLENE
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT         RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           745.091         745.091         0.00000
       MASS(LB/HR   )           79417.8         79417.8         0.00000
       ENTHALPY(BTU/HR  )      0.310005E+07   -0.819146E+07     1.37845

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

                         ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE               F                    80.0000
   SPECIFIED PRESSURE                  PSIA                 35.0000
   MAXIMUM NO. ITERATIONS                                   30
   CONVERGENCE TOLERANCE
0.000100000



                          ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    80.000
```

```
   OUTLET PRESSURE      PSIA                                  35.000
   HEAT DUTY            BTU/HR                              -0.11292E+08
   OUTLET VAPOR FRACTION                                      0.0000



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)          X(I)           Y(I)           K(I)
      ISOOCTAN         0.44261E-03    0.44261E-03    0.24937E-02
0.29519E-01
      2:4:4-01         0.30313E-03    0.30313E-03    0.15480E-02
0.26757E-01
      TRIMERS          0.66797E-02    0.66797E-02    0.14719E-03
0.11545E-03
      M-XYL-01         0.49628E-01    0.49628E-01    0.47958E-01
0.50631E-02
      O-XYL-01         0.49630E-01    0.49630E-01    0.37948E-01
0.40061E-02
      P-XYL-01         0.89332        0.89332        0.90990
0.53367E-02

 BLOCK:  M-REC    MODEL: MIXER
 -----------------------------
   INLET STREAMS:         REC1        REC2
   OUTLET STREAM:         RECYCLE
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            491.161         491.161          0.00000
       MASS(LB/HR   )            54733.2         54733.2       -
0.398805E-15
       ENTHALPY(BTU/HR  )      -0.475557E+08   -0.475557E+08
0.470012E-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:  M1       MODEL: MIXER
 -----------------------------
   INLET STREAMS:         IBUTYLE     RECGUESS    ISOOCTAN
   OUTLET STREAM:         TO-P1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

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

```
    TOTAL BALANCE
       MOLE(LBMOL/HR)           2755.36         2755.36         0.00000
       MASS(LB/HR   )           181998.         181998.
0.159912E-15
       ENTHALPY(BTU/HR  )      -0.893992E+08   -0.893992E+08   -
0.333362E-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:  M2       MODEL: MIXER
 -----------------------------
   INLET STREAMS:         R1-FEED     TO-M2
   OUTLET STREAM:         TO-R1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                       ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           10193.7         10193.7         0.00000
       MASS(LB/HR   )          0.107714E+07    0.107714E+07
0.216156E-15
       ENTHALPY(BTU/HR  )      -0.509633E+09   -0.509633E+09   -
0.233912E-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:  M3       MODEL: MIXER
 -----------------------------
   INLET STREAMS:         TO-R2       R2RCYC2
   OUTLET STREAM:         TO-R2MIX
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

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

```
       MOLE(LBMOL/HR)            37780.3         37780.1
0.319650E-05
       MASS(LB/HR   )           0.161015E+07    0.161015E+07   -
0.348916E-06
       ENTHALPY(BTU/HR  )       0.545030E+09    0.545006E+09
0.439634E-04

                      ***  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:  P-101    MODEL: PUMP
 ----------------------------
   INLET STREAM:           I8--MAKE
   OUTLET STREAM:          ISOOCTAN
   PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            3.89886         3.89886         0.00000
       MASS(LB/HR   )            445.370         445.370         0.00000
       ENTHALPY(BTU/HR  )       -433848.        -433719.       -
0.298462E-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  ***
    PRESSURE CHANGE  PSI                                   20.0000
    DRIVER EFFICIENCY                                       1.00000

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

                           ***  RESULTS  ***
    VOLUMETRIC FLOW RATE  CUFT/HR                          10.3442
    PRESSURE CHANGE  PSI                                   20.0000
    NPSH AVAILABLE   FT-LBF/LB                             46.7145
    FLUID POWER  HP                                         0.015046
    BRAKE POWER  HP                                         0.050890
    ELECTRICITY  KW                                         0.037949
    PUMP EFFICIENCY USED                                    0.29566
```

```
    NET WORK REQUIRED  HP                                   0.050890
    HEAD DEVELOPED FT-LBF/LB                               66.8912

 BLOCK:  P-102    MODEL: PUMP
 ----------------------------
   INLET STREAM:          TO-P1
   OUTLET STREAM:         TO-H1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            2755.36         2755.36          0.00000
       MASS(LB/HR   )            181998.         181998.          0.00000
       ENTHALPY(BTU/HR  )      -0.893992E+08   -0.885408E+08   -
0.960251E-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  ***
    OUTLET PRESSURE  PSIA                                 764.696
    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                       4,507.90
    PRESSURE CHANGE  PSI                                  744.696
    NPSH AVAILABLE   FT-LBF/LB                            -45.3277
    FLUID POWER  HP                                       244.146
    BRAKE POWER  HP                                       337.386
    ELECTRICITY  KW                                       251.589
    PUMP EFFICIENCY USED                                    0.72364
    NET WORK REQUIRED  HP                                 337.386
    HEAD DEVELOPED FT-LBF/LB                            2,656.12
    NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION
HEAD.

 BLOCK:  P-201    MODEL: PUMP
 ----------------------------
   INLET STREAM:          R1RECIRC
   OUTLET STREAM:         TO-R1HX
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            7438.37         7438.37          0.00000
```

```
       MASS(LB/HR   )            895140.         895140.        -
0.130053E-15
       ENTHALPY(BTU/HR  )      -0.423522E+09   -0.423402E+09   -
0.284247E-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  ***
    PRESSURE CHANGE  PSI                                  20.0000
    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                     26,022.2
    PRESSURE CHANGE  PSI                                  20.0000
    NPSH AVAILABLE   FT-LBF/LB                         2,588.59
    FLUID POWER  HP                                       37.8505
    BRAKE POWER  HP                                       47.3131
    ELECTRICITY  KW                                       35.2814
    PUMP EFFICIENCY USED                                   0.80000
    NET WORK REQUIRED  HP                                 47.3131
    HEAD DEVELOPED FT-LBF/LB                              83.7231

 BLOCK:  R-201    MODEL: RSTOIC
 ------------------------------
   INLET STREAM:          TO-R1
   OUTLET STREAM:         R1OUT
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                             IN          OUT       GENERATION   RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         10193.7       8950.74      -1242.99     -
0.356884E-15
   MASS(LB/HR   )        0.107714E+07  0.107714E+07               -
0.216156E-15
   ENTHALPY(BTU/HR  )   -0.509633E+09 -0.509633E+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  ***
   STOICHIOMETRY MATRIX:
```

```
     REACTION #   1:
      SUBSTREAM MIXED   :
      ISOBUTYL  -2.00    2:4:4-01   1.00

     REACTION #   2:
      SUBSTREAM MIXED   :
      ISOBUTYL  -3.00    TRIMERS    1.00


    REACTION CONVERSION SPECS: NUMBER=    2
      REACTION #   1:
      SUBSTREAM:MIXED    KEY COMP:ISOBUTYL CONV FRAC: 0.6000
      REACTION #   2:
      SUBSTREAM:MIXED    KEY COMP:ISOBUTYL CONV FRAC: 0.3000




    TWO    PHASE  PQ  FLASH
    SPECIFIED PRESSURE    PSIA                             764.696
    SPECIFIED HEAT DUTY   BTU/HR                             0.0
    MAXIMUM NO. ITERATIONS                                  30
    CONVERGENCE TOLERANCE                                    0.000100000
    SIMULTANEOUS REACTIONS
    GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                            ***  RESULTS  ***
    OUTLET TEMPERATURE    F                                   372.27
    OUTLET PRESSURE       PSIA                                764.70
    VAPOR FRACTION                                            0.0000



    HEAT OF REACTIONS:

      REACTION          REFERENCE          HEAT OF
      NUMBER            COMPONENT          REACTION
                                            BTU/LBMOL
       1                   ISOBUTYL          -15350.
       2                   ISOBUTYL          -16018.

    REACTION EXTENTS:

       REACTION          REACTION
       NUMBER            EXTENT
                         LBMOL/HR
       1                  745.79
       2                  248.60

    V-L PHASE EQUILIBRIUM :

       COMP              F(I)          X(I)          Y(I)          K(I)
       ISOBUTYL         0.27774E-01    0.27774E-01    0.21181
 1.4593
       ISOOCTAN         0.25109        0.25109        0.18575
 0.14155
       2:4:4-01         0.55164        0.55164        0.37820
 0.13119
```

```
      TRIMERS          0.16440        0.16440        0.89632E-02
0.10432E-01
      M-XYL-01         0.22538E-03    0.22538E-03    0.73292E-04
0.62227E-01
      O-XYL-01         0.86802E-04    0.86802E-04    0.24975E-04
0.55057E-01
      P-XYL-01         0.46277E-02    0.46277E-02    0.15206E-02
0.62877E-01
      HYDROGEN         0.14943E-03    0.14943E-03    0.21366
273.60

 BLOCK:  R-401    MODEL: RSTOIC
 ------------------------------
   INLET STREAM:          TO-R2MIX
   OUTLET STREAM:         R2OUT
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                              IN          OUT       GENERATION   RELATIVE
DIFF.
   TOTAL BALANCE
   MOLE(LBMOL/HR)         37780.1       40000.7       2220.57
0.00000
   MASS(LB/HR   )       0.161015E+07  0.161015E+07
0.144602E-15
   ENTHALPY(BTU/HR  )    0.545006E+09  0.545006E+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  ***
   STOICHIOMETRY MATRIX:

    REACTION #   1:
     SUBSTREAM MIXED   :
     2:4:4-01  -1.00    P-XYL-01   1.00    HYDROGEN   3.00

    REACTION #   2:
     SUBSTREAM MIXED   :
     2:4:4-01  -1.00    O-XYL-01   1.00    HYDROGEN   3.00

    REACTION #   3:
     SUBSTREAM MIXED   :
     2:4:4-01  -1.00    M-XYL-01   1.00    HYDROGEN   3.00


   REACTION CONVERSION SPECS: NUMBER=    3
     REACTION #   1:
     SUBSTREAM:MIXED    KEY COMP:2:4:4-01 CONV FRAC: 0.3780
     REACTION #   2:
     SUBSTREAM:MIXED    KEY COMP:2:4:4-01 CONV FRAC: 0.2100E-01
     REACTION #   3:
     SUBSTREAM:MIXED    KEY COMP:2:4:4-01 CONV FRAC: 0.2100E-01
```

```
   TWO    PHASE  PQ  FLASH
   SPECIFIED PRESSURE    PSIA                               36.6959
   SPECIFIED HEAT DUTY   BTU/HR                              0.0
   MAXIMUM NO. ITERATIONS                                   30
   CONVERGENCE TOLERANCE                                     0.000100000
   SIMULTANEOUS REACTIONS
   GENERATE COMBUSTION REACTIONS FOR FEED SPECIES          NO

                           ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                    1000.5
   OUTLET PRESSURE       PSIA                                 36.696
   VAPOR FRACTION                                             1.0000



   REACTION EXTENTS:

      REACTION          REACTION
      NUMBER            EXTENT
                        LBMOL/HR
      1                  666.17
      2                  37.009
      3                  37.009

   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      ISOBUTYL         0.12070E-01    0.74682E-03    0.12070E-01
431.17
      ISOOCTAN         0.10858        0.12305        0.10858
105.31
      2:4:4-01         0.25554E-01    0.31304E-01    0.25554E-01
133.79
      TRIMERS          0.14295E-02    0.70588E-01    0.14295E-02
38.189
      M-XYL-01         0.10718E-01    0.40204E-01    0.10718E-01
79.684
      O-XYL-01         0.10659E-01    0.46923E-01    0.10659E-01
74.913
      P-XYL-01         0.19318        0.68713        0.19318
80.184
      HYDROGEN         0.63781        0.54168E-04    0.63781
5701.1

 BLOCK:  S-301    MODEL: RADFRAC
 -------------------------------
    INLETS   - TOTRCOL  STAGE   6
    OUTLETS  - TRIOVHD  STAGE   1
               TRIBOT   STAGE   9
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN               OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1512.37         1512.37
0.150343E-15
```

```
       MASS(LB/HR   )           182000.         182000.
0.959469E-15
       ENTHALPY(BTU/HR  )      -0.861104E+08   -0.939709E+08
0.836477E-01

                      ***  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                                             9
    ALGORITHM OPTION                                          STANDARD
    ABSORBER OPTION                                           NO
    INITIALIZATION OPTION                                     STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                          NO
    INSIDE LOOP CONVERGENCE METHOD                            BROYDEN
    DESIGN SPECIFICATION METHOD                               NESTED
    MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                     100
    MAXIMUM NO. OF INSIDE LOOP ITERATIONS                       10
    MAXIMUM NUMBER OF FLASH ITERATIONS                          30
    FLASH TOLERANCE                                              0.000100000
    OUTSIDE LOOP CONVERGENCE TOLERANCE                           0.000100000

   ****   COL-SPECS   ****

    MOLAR VAPOR DIST / TOTAL DIST                                0.0
    MOLAR REFLUX RATIO                                           4.00000
    MOLAR BOTTOMS RATE             LBMOL/HR                    230.100

   ****    PROFILES   ****

    P-SPEC          STAGE   1  PRES, PSIA                     70.0000

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


   ***   COMPONENT SPLIT FRACTIONS   ***

                             OUTLET STREAMS
                             --------------
                  TRIOVHD      TRIBOT
    COMPONENT:
    ISOBUTYL    1.0000       .85574E-06
    ISOOCTAN    .99517       .48291E-02
    2:4:4-01    .99394       .60623E-02
    TRIMERS     .20000E-01   .98000
    M-XYL-01    .92350       .76499E-01
    O-XYL-01    .88599       .11401
```

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     P-XYL-01    .92511       .74895E-01
     HYDROGEN    1.0000       .56972E-14


   ***    SUMMARY OF KEY RESULTS    ***

     TOP STAGE TEMPERATURE          F                        239.567
     BOTTOM STAGE TEMPERATURE       F                        543.091
     TOP STAGE LIQUID FLOW          LBMOL/HR                 208.142
     BOTTOM STAGE LIQUID FLOW       LBMOL/HR                 251.124
     TOP STAGE VAPOR FLOW           LBMOL/HR                   0.0
     BOILUP VAPOR FLOW              LBMOL/HR                 879.103
     MOLAR REFLUX RATIO                                        0.16503
     MOLAR BOILUP RATIO                                        3.50067
     CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                    -0.270279+08
     REBOILER DUTY                  BTU/HR                     0.191675+08


   ****   MANIPULATED VARIABLES   ****

                                                    BOUNDS
CALCULATED
                                             LOWER        UPPER
VALUE
   MOLAR BOTTOMS RATE         LBMOL/HR    153.60        384.00
251.12
   MOLAR REFLUX RATIO                     0.0000        10.000
0.16503

   ****    DESIGN SPECIFICATIONS   ****

 NO  SPEC-TYPE     QUALIFIERS             UNIT       SPECIFIED
CALCULATED
                                                       VALUE
VALUE
  1  MOLE-RECOV    STREAMS: TRIBOT                    0.98000
0.98000
                   COMPS:   TRIMERS
  2  MASS-FRAC     STREAMS: TRIBOT                    0.98000
0.98000
                   COMPS:   TRIMERS

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

     DEW POINT                       0.10706E-04  STAGE=  7
     BUBBLE POINT                    0.99621E-04  STAGE=  1
     COMPONENT MASS BALANCE          0.10265E-06  STAGE=  3 COMP=TRIMERS
     ENERGY BALANCE                  0.11550E-03  STAGE=  9


   ****    PROFILES   ****

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

                                             ENTHALPY
 STAGE TEMPERATURE   PRESSURE                BTU/LBMOL          HEAT DUTY
       F             PSIA              LIQUID       VAPOR         BTU/HR
```

```
   1   239.57        70.000       -65283.      -16457.      -.27028+08
   2   340.42        72.000       -58848.      -46888.
   3   351.38        72.120       -59068.      -46293.
   4   361.06        72.240       -59372.      -45695.
   5   365.80        72.360       -59477.      -45421.
   6   367.49        72.480       -59496.      -45326.
   7   415.62        72.600       -57522.      -42499.
   8   494.16        72.720       -51476.      -35948.
   9   543.09        72.840       -46326.      -31146.       .19168+08

 STAGE     FLOW RATE                  FEED RATE                PRODUCT
RATE
            LBMOL/HR                   LBMOL/HR                  LBMOL/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1  1469.      0.000                                      1261.2428
   2  245.1      1469.
   3  173.7      1506.
   4  141.8      1435.
   5  131.3      1403.
   6  1184.      1393.      1194.1798  318.1870
   7  1009.      933.0
   8  1130.      758.0
   9  251.1      879.1                                       251.1240

    ****  MASS FLOW PROFILES  ****

 STAGE     FLOW RATE                  FEED RATE                PRODUCT
RATE
            LB/HR                      LB/HR                     LB/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1 0.1633E+06  0.000                                      .14015+06
   2 0.2840E+05 0.1633E+06
   3 0.2111E+05 0.1685E+06
   4 0.1792E+05 0.1613E+06
   5 0.1687E+05 0.1581E+06
   6 0.1530E+06 0.1570E+06  .14769+06 .34312+05
   7 0.1461E+06 0.1111E+06
   8 0.1815E+06 0.1043E+06
   9 0.4185E+05 0.1396E+06                                 .41852+05

                         ****   MOLE-X-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.33304E-01   0.29963       0.65747       0.39428E-02
0.24958E-03
      2    0.27464E-02   0.27542       0.65085       0.58969E-01
0.55330E-03
      3    0.21459E-02   0.24283       0.58099       0.16147
0.57993E-03
      4    0.20798E-02   0.21829       0.52125       0.24751
0.50095E-03
      5    0.20517E-02   0.20760       0.49466       0.28590
0.45069E-03
      6    0.20433E-02   0.20417       0.48611       0.29828
0.43226E-03
      7    0.12432E-03   0.11538       0.29587       0.57788
0.49627E-03
```

```
      8    0.49054E-05   0.35795E-01   0.96828E-01   0.86118
0.28625E-03
      9    0.14314E-06   0.73024E-02   0.20140E-01   0.97031
0.10383E-03

                         ****   MOLE-X-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.92218E-04   0.51335E-02   0.17918E-03
      2    0.23227E-03   0.11230E-01   0.61663E-07
      3    0.25295E-03   0.11736E-01   0.51717E-07
      4    0.21874E-03   0.10147E-01   0.54382E-07
      5    0.19471E-03   0.91434E-02   0.55709E-07
      6    0.18549E-03   0.87765E-02   0.56221E-07
      7    0.23496E-03   0.10011E-01   0.24758E-10
      8    0.14930E-03   0.57607E-02   0.11456E-13
      9    0.59598E-04   0.20873E-02   0.51271E-17

                         ****   MOLE-Y-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.16684       0.97386E-01   0.19969       0.37166E-04
0.26442E-04
      2    0.33304E-01   0.29963       0.65747       0.39428E-02
0.24958E-03
      3    0.28331E-01   0.29569       0.65639       0.12898E-01
0.29900E-03
      4    0.29533E-01   0.29275       0.64821       0.23008E-01
0.28956E-03
      5    0.30148E-01   0.29141       0.64370       0.28558E-01
0.27498E-03
      6    0.30357E-01   0.29095       0.64212       0.30527E-01
0.26854E-03
      7    0.25931E-02   0.25716       0.61152       0.11740
0.52066E-03
      8    0.16546E-03   0.15119       0.38722       0.44787
0.62628E-03
      9    0.62658E-05   0.43934E-01   0.11873       0.83000
0.33837E-03

                         ****   MOLE-Y-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.83992E-05   0.55734E-03   0.53546
      2    0.92218E-04   0.51335E-02   0.17918E-03
      3    0.11501E-03   0.61256E-02   0.15003E-03
      4    0.11167E-03   0.59326E-02   0.15750E-03
      5    0.10500E-03   0.56402E-02   0.16108E-03
      6    0.10188E-03   0.55115E-02   0.16229E-03
      7    0.21937E-03   0.10577E-01   0.71352E-07
      8    0.29305E-03   0.12636E-01   0.32960E-10
      9    0.17493E-03   0.68100E-02   0.14727E-13

                         ****   K-VALUES           ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1     5.0097        0.32502       0.30372       0.94252E-02
0.10594
      2     12.126         1.0879        1.0102       0.66862E-01
0.45107
      3     13.202         1.2177        1.1298       0.79877E-01
0.51559
```

```
      4     14.200        1.3411        1.2436       0.92960E-01
0.57802
      5     14.694        1.4037        1.3013       0.99889E-01
0.61014
      6     14.857        1.4250        1.3209       0.10235
0.62124
      7     20.857        2.2288        2.0668       0.20317
1.0492
      8     33.731        4.2237        3.9990       0.52007
2.1878
      9     43.775        6.0164        5.8954       0.85540
3.2588

                         ****   K-VALUES           ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.91075E-01   0.10857        2988.9
      2    0.39703       0.45712        2905.8
      3    0.45467       0.52195        2901.0
      4    0.51053       0.58463        2896.2
      5    0.53930       0.61686        2891.4
      6    0.54926       0.62799        2886.6
      7    0.93368        1.0565        2881.8
      8     1.9628        2.1936        2877.1
      9     2.9352        3.2626        2872.3

                         ****   MASS-X-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.16816E-01   0.30802      0.66396       0.59725E-02
0.23846E-03
      2    0.13301E-02   0.27156      0.63042       0.85677E-01
0.50704E-03
      3    0.99042E-03   0.22817      0.53629       0.22357
0.50646E-03
      4    0.92350E-03   0.19734      0.46290       0.32970
0.42090E-03
      5    0.89584E-03   0.18454      0.43197       0.37450
0.37236E-03
      6    0.88738E-03   0.18053      0.42224       0.38863
0.35523E-03
      7    0.48174E-04   0.91025E-01  0.22929       0.67176
0.36386E-03
      8    0.17141E-05   0.25465E-01  0.67669E-01   0.90277
0.18927E-03
      9    0.48189E-07   0.50052E-02  0.13561E-01   0.98000
0.66145E-04

                         ****   MASS-X-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.88109E-04   0.49047E-02  0.32507E-05
      2    0.21285E-03   0.10291E-01  0.10730E-08
      3    0.22091E-03   0.10249E-01  0.85759E-09
      4    0.18378E-03   0.85259E-02  0.86758E-09
      5    0.16087E-03   0.75543E-02  0.87395E-09
      6    0.15243E-03   0.72124E-02  0.87726E-09
      7    0.17227E-03   0.73403E-02  0.34467E-12
      8    0.98720E-04   0.38090E-02  0.14382E-15
      9    0.37966E-04   0.13297E-02  0.62017E-19

                         ****   MASS-Y-PROFILE     ****
```

```
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.21254       0.25259       0.50879       0.14204E-03
0.63741E-04
      2    0.16816E-01   0.30802       0.66396       0.59725E-02
0.23846E-03
      3    0.14207E-01   0.30188       0.65831       0.19403E-01
0.28371E-03
      4    0.14744E-01   0.29757       0.64724       0.34461E-01
0.27354E-03
      5    0.15015E-01   0.29547       0.64117       0.42668E-01
0.25914E-03
      6    0.15106E-01   0.29475       0.63903       0.45570E-01
0.25284E-03
      7    0.12216E-02   0.24663       0.57614       0.16592
0.46410E-03
      8    0.67491E-04   0.12555       0.31588       0.54804
0.48336E-03
      9    0.22134E-05   0.31598E-01   0.83888E-01   0.87962
0.22618E-03

                         ****   MASS-Y-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.20247E-04   0.13435E-02   0.24509E-01
      2    0.88109E-04   0.49047E-02   0.32507E-05
      3    0.10913E-03   0.58124E-02   0.27031E-05
      4    0.10549E-03   0.56044E-02   0.28252E-05
      5    0.98954E-04   0.53152E-02   0.28823E-05
      6    0.95926E-04   0.51894E-02   0.29015E-05
      7    0.19554E-03   0.94278E-02   0.12076E-08
      8    0.22618E-03   0.97529E-02   0.48302E-12
      9    0.11693E-03   0.45521E-02   0.18691E-15



                    ********************************
                    ***** HYDRAULIC PARAMETERS *****
                    ********************************


       *** DEFINITIONS ***

        MARANGONI INDEX = SIGMA - SIGMATO
        FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
        QR = QV*SQRT(RHOV/(RHOL-RHOV))
        F FACTOR = QV*SQRT(RHOV)
          WHERE:
          SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
          SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
          ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
          MV IS THE MASS FLOW OF VAPOR TO THE STAGE
          RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
          RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
          QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                     TEMPERATURE
                         F
 STAGE       LIQUID FROM       VAPOR TO
```

```
    1         239.57            340.42
    2         340.42            351.38
    3         351.38            361.06
    4         361.06            365.80
    5         365.80            367.49
    6         367.49            400.21
    7         415.62            494.16
    8         494.16            543.09
    9         543.09            543.09


             MASS FLOW                VOLUME FLOW         MOLECULAR
WEIGHT
              LB/HR                     CUFT/HR
 STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR
TO
    1  0.16328E+06 0.16328E+06  4229.1     0.17523E+06  111.12
111.12
    2   28401.     0.16855E+06  805.37     0.18180E+06  115.85
111.89
    3   21112.     0.16126E+06  595.26     0.17495E+06  121.57
112.38
    4   17917.     0.15806E+06  503.44     0.17176E+06  126.36
112.66
    5   16871.     0.15702E+06  473.60     0.17054E+06  128.50
112.76
    6  0.15298E+06 0.14544E+06  4293.9     0.15930E+06  129.19
116.24
    7  0.14612E+06 0.10427E+06  4120.2     0.10670E+06  144.80
137.56
    8  0.18148E+06 0.13963E+06  5318.6     0.12987E+06  160.57
158.83
    9   41852.      0.0000      1277.2      0.0000      166.66


               DENSITY                  VISCOSITY         SURFACE TENSION
               LB/CUFT                   CP                  DYNE/CM
 STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO      LIQUID FROM
    1   38.608      0.93181      0.16267      0.93026E-02    11.523
    2   35.264      0.92712      0.12476      0.93876E-02    7.3629
    3   35.467      0.92177      0.13069      0.94660E-02    7.4777
    4   35.589      0.92025      0.13540      0.95027E-02    7.5443
    5   35.623      0.92070      0.13730      0.95158E-02    7.5562
    6   35.628      0.91302      0.13783      0.97026E-02    7.5532
    7   35.465      0.97726      0.14544      0.97660E-02    7.2051
    8   34.121       1.0751      0.13978      0.94360E-02    5.8250
    9   32.769                   0.13226                     4.6982


       MARANGONI INDEX   FLOW PARAM          QR          REDUCED F-FACTOR
 STAGE    DYNE/CM                          CUFT/HR       (LB-CUFT)**.5/HR
    1                    0.15535           27557.          0.16915E+06
    2   -4.1606          0.27322E-01       29873.          0.17505E+06
    3   0.11484          0.21106E-01       28577.          0.16796E+06
    4   0.66623E-01      0.18227E-01       27984.          0.16477E+06
    5   0.11889E-01      0.17274E-01       27779.          0.16364E+06
    6   -.16997          0.16838           25834.          0.15221E+06
    7   -.34806          0.23263           17961.          0.10548E+06
    8   -1.3801          0.23071           23425.          0.13466E+06
    9   -1.1268                            0.0000           0.0000
```

```
             ************************************
             ***** TRAY SIZING CALCULATIONS *****
             ************************************


*******************
*** SECTION   1 ***
*******************

STARTING STAGE NUMBER                                         2
ENDING STAGE NUMBER                                           8
FLOODING CALCULATION METHOD                               GLITSCH6

DESIGN PARAMETERS
-----------------
PEAK CAPACITY FACTOR                                      1.00000
SYSTEM FOAMING FACTOR                                     1.00000
FLOODING FACTOR                                           0.80000
MINIMUM COLUMN DIAMETER         FT                        1.00000
MINIMUM DC AREA/COLUMN AREA                               0.100000
HOLE AREA/ACTIVE AREA                                     0.100000

TRAY SPECIFICATIONS
-------------------
TRAY TYPE                                                 SIEVE
NUMBER OF PASSES                                              1
TRAY SPACING                    FT                        1.50000


        ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER                                   2
COLUMN DIAMETER                 FT                        6.59550
DC AREA/COLUMN AREA                                       0.100000
DOWNCOMER VELOCITY              FT/SEC                    0.065480
FLOW PATH LENGTH                FT                        4.53143
SIDE DOWNCOMER WIDTH            FT                        1.03204
SIDE WEIR LENGTH                FT                        4.79237
CENTER DOWNCOMER WIDTH          FT                        0.0
CENTER WEIR LENGTH              FT                        MISSING
OFF-CENTER DOWNCOMER WIDTH      FT                        0.0
OFF-CENTER SHORT WEIR LENGTH    FT                        MISSING
OFF-CENTER LONG WEIR LENGTH     FT                        MISSING
TRAY CENTER TO OCDC CENTER      FT                        0.0


                      **** SIZING PROFILES ****

   STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
              FT            SQFT         SQFT           SQFT
      2       6.5955        34.165       27.332        3.4165
      3       6.5955        34.165       27.332        3.4165
      4       6.5955        34.165       27.332        3.4165
      5       6.5955        34.165       27.332        3.4165
      6       6.5955        34.165       27.332        3.4165
      7       6.5955        34.165       27.332        3.4165
```

```
         8       6.5955        34.165       27.332        3.4165


                **** ADDITIONAL SIZING PROFILES ****

       FLOODING                                DC BACKUP/
 STAGE FACTOR      PRES. DROP  DC BACKUP   (TSPC+WHT)
                    PSI         FT
   2     80.00      0.8851E-01  0.6717       41.33
   3     75.68      0.8288E-01  0.6121       37.67
   4     73.73      0.8039E-01  0.5864       36.09
   5     73.06      0.7954E-01  0.5779       35.56
   6     86.37      0.8968E-01   1.522       93.68
   7     65.59      0.7117E-01   1.374       84.56
   8     85.53      0.8442E-01   1.966       121.0

       HEIGHT      DC REL      TR LIQ REL  FRA APPR TO
 STAGE OVER WEIR   FROTH DENS  FROTH DENS  SYS LIMIT
        FT
   2    0.1793      0.5876      0.2004       60.86
   3    0.1423      0.5884      0.2055       58.01
   4    0.1255      0.5889      0.2079       56.70
   5    0.1199      0.5891      0.2088       56.27
   6    0.7478      0.5891      0.2190       52.89
   7    0.4868      0.5882      0.2848       37.28
   8    0.8150      0.5815      0.2384       51.34

 BLOCK:  S-501    MODEL: RADFRAC
 -------------------------------
    INLETS   - TOXYLCL  STAGE   5
    OUTLETS  - XYOVHD   STAGE   1
               REC1     STAGE   1
               XYLBOT   STAGE  16
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                       ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)           3481.69         3481.69       -
0.117550E-14
       MASS(LB/HR   )           140148.         140148.       -
0.269964E-14
       ENTHALPY(BTU/HR  )      -0.209937E+08   -0.425007E+08    0.506039

                       ***  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                                                      16
 ALGORITHM OPTION                                                    STANDARD
 INITIALIZATION OPTION                                               STANDARD
 HYDRAULIC PARAMETER CALCULATIONS                                    NO
 INSIDE LOOP CONVERGENCE METHOD                                      NEWTON
 DESIGN SPECIFICATION METHOD                                         NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                                80
 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   ****

 CONDENSER TEMPERATURE          F                                    100.0000
 MASS REFLUX RATIO                                                     6.00000
 MASS BOTTOMS RATE              LB/HR                              75,000.0

****    PROFILES   ****

 P-SPEC          STAGE   1  PRES, PSIA                                39.0000

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


***   COMPONENT SPLIT FRACTIONS   ***

                                OUTLET STREAMS
                                --------------
               XYOVHD       REC1         XYLBOT
 COMPONENT:
 ISOBUTYL     .91030       .89701E-01   0.0000
 ISOOCTAN     .21423       .78490        .87239E-03
 2:4:4-01     .19905       .79841        .25386E-02
 TRIMERS      .60228E-09   .40675E-06   1.0000
 M-XYL-01     .45444E-03   .86795E-02   .99087
 O-XYL-01     .14302E-03   .33942E-02   .99646
 P-XYL-01     .53843E-03   .98665E-02   .98960
 HYDROGEN     .99997       .29935E-04   0.0000


***    SUMMARY OF KEY RESULTS    ***

 TOP STAGE TEMPERATURE          F                                    100.0000
 BOTTOM STAGE TEMPERATURE       F                                    366.882
 TOP STAGE LIQUID FLOW          LBMOL/HR                           3,896.41
 BOTTOM STAGE LIQUID FLOW       LBMOL/HR                             745.091
 TOP STAGE VAPOR FLOW           LBMOL/HR                           2,357.93
 BOILUP VAPOR FLOW              LBMOL/HR                           5,697.93
 MOLAR REFLUX RATIO                                                    1.42382
 MOLAR BOILUP RATIO                                                    7.64730
 CONDENSER DUTY (W/O SUBCOOL)   BTU/HR                                -0.101916+09
 REBOILER DUTY                  BTU/HR                                 0.804090+08


****   MANIPULATED VARIABLES   ****
```

```
                                                 BOUNDS
CALCULATED
                                          LOWER         UPPER
VALUE
   MASS BOTTOMS RATE          LB/HR       25590.       0.11000E+06
79418.
   MASS REFLUX RATIO                     0.70000        20.000
7.2566

   ****    DESIGN SPECIFICATIONS   ****

 NO  SPEC-TYPE     QUALIFIERS              UNIT       SPECIFIED
CALCULATED
                                                        VALUE
VALUE
  1  MASS-RECOV    STREAMS: XYLBOT                     0.99000
0.99000
                   COMPS:   M-XYL-01
                            O-XYL-01
                            P-XYL-01
  2  MASS-RECOV    STREAMS: XYLBOT                     0.99000
0.99000
                   COMPS:   M-XYL-01
                            O-XYL-01
                            P-XYL-01

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

    DEW POINT                       0.22682E-10  STAGE=  5
    BUBBLE POINT                    0.11424E-06  STAGE=  5
    COMPONENT MASS BALANCE          0.11185E-10  STAGE=  8 COMP=ISOBUTYL
    ENERGY BALANCE                  0.72459E-07  STAGE=  6


   ****    PROFILES   ****

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

                                          ENTHALPY
 STAGE TEMPERATURE   PRESSURE             BTU/LBMOL          HEAT DUTY
       F             PSIA           LIQUID       VAPOR        BTU/HR

   1   100.00        39.000       -98123.      -3581.3      -.10192+09
   2   258.25        43.000       -84939.      -49150.
   3   273.30        43.120       -77248.      -54056.
   4   281.59        43.240       -64573.      -49160.
   5   293.32        43.360       -46819.      -39377.
   6   326.58        43.480       -32532.      -38624.
  15   366.15        44.560        4412.0       18428.
  16   366.88        44.680        4160.6       18557.       .80409+08

 STAGE     FLOW RATE                  FEED RATE                PRODUCT
RATE
            LBMOL/HR                   LBMOL/HR                  LBMOL/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED       LIQUID
VAPOR
   1  4275.      2358.                                       378.6703
2357.9266
```

```
   2  6614.      6633.
   3  6795.      9350.
   4  6512.      9531.
   5  5922.      9248.                               3481.6881
   6  6486.      5177.
  15  6443.      5703.
  16  745.1      5698.                                                745.0912

    ****  MASS FLOW PROFILES  ****

 STAGE     FLOW RATE                        FEED RATE                 PRODUCT
RATE
            LB/HR                            LB/HR                          LB/HR
       LIQUID     VAPOR       LIQUID    VAPOR    MIXED      LIQUID
VAPOR
   1 0.4835E+06 0.1790E+05                                             .42829+05
.17902+05
   2 0.7497E+06 0.5014E+06
   3 0.7667E+06 0.8104E+06
   4 0.7281E+06 0.8274E+06
   5 0.6536E+06 0.7888E+06                             .14015+06
   6 0.7091E+06 0.5742E+06
  15 0.6848E+06 0.6057E+06
  16 0.7942E+05 0.6054E+06                                             .79418+05

                         ****   MOLE-X-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.99546E-02   0.78357       0.18759       0.53461E-08
0.85538E-03
      2    0.12430E-02   0.75497       0.19311       0.14747E-06
0.23550E-02
      3    0.47647E-03   0.69017       0.18805       0.32576E-05
0.57297E-02
      4    0.39089E-03   0.57681       0.16674       0.61281E-04
0.12269E-01
      5    0.35732E-03   0.42105       0.12835       0.90545E-03
0.21811E-01
      6    0.22786E-04   0.31029       0.10173       0.84991E-03
0.28454E-01
     15    0.41424E-16   0.95062E-03   0.60607E-03   0.17441E-02
0.49647E-01
     16    0.19418E-17   0.44261E-03   0.30313E-03   0.66797E-02
0.49628E-01

                         ****   MOLE-X-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.33264E-03   0.17525E-01   0.17555E-03
      2    0.10588E-02   0.47198E-01   0.68829E-04
      3    0.29606E-02   0.11256       0.48958E-04
      4    0.72803E-02   0.23640       0.48159E-04
      5    0.14839E-01   0.41264       0.49769E-04
      6    0.17920E-01   0.54073       0.11832E-07
     15    0.44502E-01   0.90255        0.0000
     16    0.49630E-01   0.89332       0.63123E-24

                         ****   MOLE-Y-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
```

```
      1    0.16223E-01   0.34345E-01   0.75107E-02   0.12713E-11
0.71923E-05
      2    0.12183E-01   0.51723       0.12357       0.34461E-08
0.55386E-03
      3    0.53736E-02   0.57440       0.14608       0.10453E-06
0.17022E-02
      4    0.47487E-02   0.53164       0.14337       0.23225E-05
0.41204E-02
      5    0.48191E-02   0.44697       0.12700       0.43148E-04
0.86754E-02
      6    0.40875E-03   0.48159       0.14677       0.74366E-04
0.17807E-01
     15    0.99104E-15   0.21744E-02   0.12851E-02   0.28443E-03
0.49384E-01
     16    0.46587E-16   0.10170E-02   0.64568E-03   0.10987E-02
0.49649E-01

                         ****   MOLE-Y-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.22509E-05   0.15359E-03   0.94176
      2    0.21519E-03   0.11350E-01   0.33489
      3    0.76297E-03   0.34133E-01   0.23755
      4    0.21244E-02   0.80973E-01   0.23302
      5    0.51403E-02   0.16721       0.24015
      6    0.98315E-02   0.34346       0.56932E-04
     15    0.39065E-01   0.90781        0.0000
     16    0.43832E-01   0.90376       0.29558E-20

                         ****   K-VALUES           ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1     1.6297       0.43832E-01   0.40038E-01   0.23779E-03
0.84083E-02
      2     9.8010       0.68510       0.63993       0.23368E-01
0.23518
      3     11.278       0.83226       0.77681       0.32086E-01
0.29709
      4     12.148       0.92169       0.85984       0.37900E-01
0.33584
      5     13.487        1.0616       0.98948       0.47654E-01
0.39776
      6     17.939        1.5520        1.4427       0.87498E-01
0.62583
     15     23.924        2.2873        2.1204       0.16308
0.99471
     16     23.992        2.2978        2.1301       0.16449
1.0004

                         ****   K-VALUES           ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.67669E-02   0.87638E-02    5364.6
      2    0.20324       0.24047        4865.6
      3    0.25770       0.30325        4852.1
      4    0.29180       0.34252        4838.6
      5    0.34640       0.40522        4825.2
      6    0.54864       0.63518        4811.9
     15    0.87782        1.0058        4695.3
     16    0.88316        1.0117        4682.7

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

```
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.49382E-02   0.79138       0.18612       0.79562E-08
0.80292E-03
      2    0.61528E-03   0.76081       0.19117       0.21898E-06
0.22057E-02
      3    0.23691E-03   0.69867       0.18701       0.48593E-05
0.53908E-02
      4    0.19616E-03   0.58932       0.16735       0.92258E-04
0.11650E-01
      5    0.18164E-03   0.43577       0.13049       0.13809E-02
0.20980E-01
      6    0.11693E-04   0.32418       0.10441       0.13084E-02
0.27629E-01
     15    0.21867E-16   0.10217E-02   0.63987E-03   0.27621E-02
0.49591E-01
     16    0.10222E-17   0.47435E-03   0.31913E-03   0.10549E-01
0.49432E-01

                         ****   MASS-X-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.31224E-03   0.16450E-01   0.31289E-05
      2    0.99169E-03   0.44206E-01   0.12241E-05
      3    0.27855E-02   0.10590       0.87462E-06
      4    0.69131E-02   0.22448       0.86832E-06
      5    0.14274E-01   0.39692       0.90900E-06
      6    0.17401E-01   0.52505       0.21814E-09
     15    0.44452E-01   0.90153        0.0000
     16    0.49434E-01   0.88979       0.11938E-25

                         ****   MASS-Y-PROFILE     ****
   STAGE     ISOBUTYL      ISOOCTAN      2:4:4-01      TRIMERS       M-
XYL-01
      1    0.11990       0.51676       0.11101       0.28185E-10
0.10058E-03
      2    0.90423E-02   0.78157       0.18343       0.76731E-08
0.77784E-03
      3    0.34786E-02   0.75704       0.18913       0.20299E-06
0.20851E-02
      4    0.30691E-02   0.69954       0.18532       0.45031E-05
0.50389E-02
      5    0.31702E-02   0.59864       0.16709       0.85155E-04
0.10799E-01
      6    0.20677E-03   0.49598       0.14849       0.11285E-03
0.17045E-01
     15    0.52353E-15   0.23386E-02   0.13578E-02   0.45076E-03
0.49364E-01
     16    0.24602E-16   0.10935E-02   0.68195E-03   0.17406E-02
0.49611E-01

                         ****   MASS-Y-PROFILE     ****
   STAGE     O-XYL-01      P-XYL-01      HYDROGEN
      1    0.31477E-04   0.21477E-02   0.25006
      2    0.30222E-03   0.15940E-01   0.89304E-02
      3    0.93457E-03   0.41810E-01   0.55250E-02
      4    0.25979E-02   0.99025E-01   0.54110E-02
      5    0.63985E-02   0.20814       0.56761E-02
      6    0.94106E-02   0.32875       0.10347E-05
     15    0.39049E-01   0.90744        0.0000
     16    0.43798E-01   0.90307       0.56082E-22
```

```
                    ********************************
                    ***** HYDRAULIC PARAMETERS *****
                    ********************************


       *** DEFINITIONS ***

        MARANGONI INDEX = SIGMA - SIGMATO
        FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
        QR = QV*SQRT(RHOV/(RHOL-RHOV))
        F FACTOR = QV*SQRT(RHOV)
          WHERE:
          SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
          SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
          ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
          MV IS THE MASS FLOW OF VAPOR TO THE STAGE
          RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
          RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
          QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE


                     TEMPERATURE
                         F
 STAGE       LIQUID FROM      VAPOR TO
    1         100.00           258.25
    2         258.25           273.30
    3         273.30           281.59
    4         281.59           293.32
    5         293.32           318.70
    6         326.58           338.39
   15         366.15           366.88
   16         366.88           366.88


             MASS FLOW                VOLUME FLOW         MOLECULAR
WEIGHT
              LB/HR                    CUFT/HR
 STAGE LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR TO   LIQUID FROM  VAPOR
TO
    1  0.48353E+06 0.50143E+06  11295.     0.11884E+07  113.10
75.596
    2  0.74968E+06 0.81041E+06  19774.     0.17056E+07  113.35
86.673
    3  0.76671E+06 0.82744E+06  20182.     0.17534E+07  112.84
86.814
    4  0.72806E+06 0.78879E+06  18705.     0.17236E+07  111.81
85.289
    5  0.65361E+06 0.71434E+06  16185.     0.16680E+07  110.37
82.502
    6  0.70914E+06 0.62972E+06  17489.     0.11277E+07  109.34
109.69
   15  0.68481E+06 0.60539E+06  15616.     0.11312E+07  106.29
106.25
   16   79418.      0.0000      1814.1      0.0000      106.59
```

```
               DENSITY                      VISCOSITY          SURFACE TENSION
               LB/CUFT                        CP                     DYNE/CM
STAGE LIQUID FROM  VAPOR TO     LIQUID FROM  VAPOR TO       LIQUID FROM
   1   42.807      0.42193      0.37428      0.90872E-02    17.835
   2   37.913      0.47514      0.18041      0.89518E-02    10.420
   3   37.990      0.47190      0.17351      0.90449E-02    10.241
   4   38.924      0.45765      0.17482      0.92232E-02    10.805
   5   40.383      0.42827      0.17753      0.95929E-02    11.585
   6   40.549      0.55843      0.16446      0.91921E-02    10.874
  15   43.853      0.53519      0.16644      0.96173E-02    11.501
  16   43.779                   0.16655                     11.478


      MARANGONI INDEX   FLOW PARAM         QR           REDUCED F-FACTOR
STAGE    DYNE/CM                         CUFT/HR       (LB-CUFT)**.5/HR
   1                    0.95735E-01     0.11857E+06     0.77195E+06
   2   -7.4155          0.10356         0.19215E+06     0.11757E+07
   3   -.17874          0.10327         0.19665E+06     0.12045E+07
   4   0.56427          0.10008         0.18800E+06     0.11660E+07
   5   0.77936          0.94226E-01     0.17269E+06     0.10916E+07
   6   -.71014          0.13215         0.13326E+06     0.84268E+06
  15   -.92641E-02      0.12496         0.12573E+06     0.82753E+06
  16   -.23413E-01                       0.0000          0.0000




                ************************************
                ***** TRAY SIZING CALCULATIONS *****
                ************************************


   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                                             2
   ENDING STAGE NUMBER                                              15
   FLOODING CALCULATION METHOD                                 GLITSCH6

   DESIGN PARAMETERS
   -----------------
   PEAK CAPACITY FACTOR                                        1.00000
   SYSTEM FOAMING FACTOR                                       1.00000
   FLOODING FACTOR                                             0.80000
   MINIMUM COLUMN DIAMETER          FT                         1.00000
   MINIMUM DC AREA/COLUMN AREA                                 0.100000
   HOLE AREA/ACTIVE AREA                                       0.100000

   TRAY SPECIFICATIONS
   -------------------
   TRAY TYPE                                                   SIEVE
   NUMBER OF PASSES                                                 1
   TRAY SPACING                     FT                         2.00000


        ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

   STAGE WITH MAXIMUM DIAMETER                                      3
   COLUMN DIAMETER                  FT                        19.4443
```

```
   DC AREA/COLUMN AREA                                       0.100000
   DOWNCOMER VELOCITY             FT/SEC                     0.18879
   FLOW PATH LENGTH               FT                        13.3592
   SIDE DOWNCOMER WIDTH           FT                         3.04256
   SIDE WEIR LENGTH               FT                        14.1285
   CENTER DOWNCOMER WIDTH         FT                         0.0
   CENTER WEIR LENGTH             FT                         MISSING
   OFF-CENTER DOWNCOMER WIDTH     FT                         0.0
   OFF-CENTER SHORT WEIR LENGTH   FT                         MISSING
   OFF-CENTER LONG WEIR LENGTH    FT                         MISSING
   TRAY CENTER TO OCDC CENTER     FT                         0.0


                         **** SIZING PROFILES ****

      STAGE    DIAMETER      TOTAL AREA   ACTIVE AREA   SIDE DC AREA
                 FT            SQFT         SQFT           SQFT
         2       19.444        296.94       237.56        29.694
         3       19.444        296.94       237.56        29.694
         4       19.444        296.94       237.56        29.694
         5       19.444        296.94       237.56        29.694
         6       19.444        296.94       237.56        29.694
         7       19.444        296.94       237.56        29.694
         8       19.444        296.94       237.56        29.694
         9       19.444        296.94       237.56        29.694
        10       19.444        296.94       237.56        29.694
        11       19.444        296.94       237.56        29.694
        12       19.444        296.94       237.56        29.694
        13       19.444        296.94       237.56        29.694
        14       19.444        296.94       237.56        29.694
        15       19.444        296.94       237.56        29.694


              **** ADDITIONAL SIZING PROFILES ****

      FLOODING                            DC BACKUP/
STAGE FACTOR      PRES. DROP  DC BACKUP   (TSPC+WHT)
                   PSI         FT
  2     78.26      0.9431E-01   1.676       77.33
  3     80.00      0.9606E-01   1.718       79.31
  4     75.60      0.9414E-01   1.566       72.28
  5     67.95      0.9016E-01   1.331       61.45
  6     59.85      0.8709E-01   1.439       66.43
  7     57.78      0.8762E-01   1.367       63.11
  8     56.55      0.8829E-01   1.323       61.08
  9     55.90      0.8882E-01   1.299       59.97
 10     55.57      0.8917E-01   1.287       59.40
 11     55.40      0.8937E-01   1.281       59.13
 12     55.30      0.8948E-01   1.278       59.00
 13     55.25      0.8953E-01   1.277       58.95
 14     55.21      0.8956E-01   1.277       58.93
 15     55.16      0.8954E-01   1.276       58.92

      HEIGHT      DC REL      TR LIQ REL  FRA APPR TO
STAGE OVER WEIR   FROTH DENS  FROTH DENS  SYS LIMIT
       FT
  2    0.6692      0.5974      0.2376       40.95
  3    0.6879      0.5976      0.2336       42.11
  4    0.6399      0.5995      0.2390       39.87
  5    0.5571      0.6019      0.2507       36.17
```

```
   6    0.5146      0.6020      0.3027       28.65
   7    0.4946      0.6034      0.3053       27.84
   8    0.4830      0.6043      0.3061       27.44
   9    0.4770      0.6047      0.3061       27.26
  10    0.4740      0.6050      0.3060       27.19
  11    0.4725      0.6051      0.3060       27.15
  12    0.4717      0.6052      0.3060       27.13
  13    0.4713      0.6052      0.3062       27.11
  14    0.4710      0.6052      0.3063       27.09
  15    0.4705      0.6052      0.3067       27.05

 BLOCK:  S-502    MODEL: FLASH2
 ------------------------------
   INLET STREAM:           TO-F1
   OUTLET VAPOR STREAM:    EXHAUST
   OUTLET LIQUID STREAM:   REC2
   PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN                OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            2357.93         2357.93          0.00000
       MASS(LB/HR   )            17901.6         17901.6       -
0.203220E-15
       ENTHALPY(BTU/HR  )       -536402.       -0.113334E+08    0.952671

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

                         ***  INPUT DATA  ***
   TWO    PHASE  TP  FLASH
   SPECIFIED TEMPERATURE F                                   40.0000
   PRESSURE DROP         PSI                                  0.0
   MAXIMUM NO. ITERATIONS                                    30
   CONVERGENCE TOLERANCE                                      0.000100000

                          ***  RESULTS  ***
   OUTLET TEMPERATURE    F                                     40.000
   OUTLET PRESSURE       PSIA                                  300.00
   HEAT DUTY             BTU/HR                              -0.10797E+08
   VAPOR FRACTION                                             0.95229



   V-L PHASE EQUILIBRIUM :

      COMP              F(I)           X(I)           Y(I)           K(I)
      ISOBUTYL        0.16223E-01    0.13607        0.10220E-01
0.75108E-01
      ISOOCTAN        0.34345E-01    0.70465        0.76441E-03
0.10848E-02
      2:4:4-01        0.75107E-02    0.15446        0.14910E-03
0.96530E-03
      TRIMERS         0.12713E-11    0.26646E-10    0.53733E-16
0.20165E-05
```

```
      M-XYL-01         0.71923E-05    0.15031E-03    0.22349E-07
0.14868E-03
      O-XYL-01         0.22509E-05    0.47075E-04    0.53563E-08
0.11378E-03
      P-XYL-01         0.15359E-03    0.32093E-02    0.50170E-06
0.15632E-03
      HYDROGEN         0.94176        0.14179E-02    0.98887
697.40

 BLOCK:  S1       MODEL: FSPLIT
 ------------------------------
   INLET STREAM:          R1OUT
   OUTLET STREAMS:        R1RECIRC    TO-V1
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT          RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            8950.74         8950.74          0.00000
       MASS(LB/HR   )           0.107714E+07    0.107714E+07      0.00000
       ENTHALPY(BTU/HR  )      -0.509633E+09   -0.509633E+09
0.233912E-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  ***

  MASS-FLOW  (LB/HR   )            STRM=R1RECIRC FLOW=   895,140.
KEY= 0

                           ***  RESULTS  ***

  STREAM= R1RECIRC       SPLIT=          0.83103     KEY=  0    STREAM-
ORDER=   1
          TO-V1                          0.16897           0
2

 BLOCK:  S2       MODEL: FSPLIT
 ------------------------------
   INLET STREAM:          TO-S2
   OUTLET STREAMS:        R2TOXYLC    R2RECYCL
   PROPERTY OPTION SET:   NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT          RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            40000.7         40000.7          0.00000
       MASS(LB/HR   )           0.161015E+07    0.161015E+07      0.00000
       ENTHALPY(BTU/HR  )       0.573019E+09    0.573019E+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  ***

  MASS-FLOW  (LB/HR   )            STRM=R2RECYCL FLOW= 1,470,000.
KEY= 0

                           ***  RESULTS  ***

  STREAM= R2TOXYLC       SPLIT=          0.087041    KEY=  0    STREAM-
ORDER=   2
          R2RECYCL                       0.91296           0
1

 BLOCK:  V-301    MODEL: VALVE
 -----------------------------
   INLET STREAM:           TO-V1
   OUTLET STREAM:          TOTRCOL
   PROPERTY OPTION SET:    NRTL      RENON (NRTL) / IDEAL GAS

                      ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE
DIFF.
    TOTAL BALANCE
       MOLE(LBMOL/HR)            1512.37         1512.37         0.00000
       MASS(LB/HR   )            182000.         182000.       -
0.159912E-15
       ENTHALPY(BTU/HR  )      -0.861104E+08   -0.861104E+08     0.00000

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

                          ***  INPUT DATA  ***

    VALVE OUTLET PRESSURE     PSIA                         80.0000
    VALVE FLOW COEF CALC.                                 NO

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

                          ***  RESULTS  ***

    VALVE PRESSURE DROP       PSI                         684.696
```

```
 EXHAUST FDWU I8--MAKE IBUTYLE ISOOCTAN
 --------------------------------------

 STREAM ID               EXHAUST    FDWU       I8--MAKE   IBUTYLE
ISOOCTAN
 FROM :                  S-502      ----       ----       ----       P-
101
 TO   :                  ----       ----       P-101      M1         M1

 SUBSTREAM: MIXED
 PHASE:                  VAPOR      LIQUID     LIQUID     LIQUID
LIQUID
 COMPONENTS: LBMOL/HR
   ISOBUTYL              22.9476    41.1714     0.0     2260.3031     0.0
   ISOOCTAN               1.7164   378.8524     3.8989     0.0
3.8989
   2:4:4-01               0.3348   786.6263     0.0        0.0        0.0
   TRIMERS              1.2065-13  246.8262     0.0        0.0        0.0
   M-XYL-01             5.0184-05    1.6059     0.0        0.0        0.0
   O-XYL-01             1.2027-05    0.6429     0.0        0.0        0.0
   P-XYL-01             1.1265-03   32.8057     0.0        0.0        0.0
   HYDROGEN             2220.4364  6.2797-02    0.0        0.0        0.0
 TOTAL FLOW:
   LBMOL/HR             2245.4364  1488.5937     3.8989  2260.3031
3.8989
   LB/HR                5997.4296  1.7913+05   445.3700  1.2682+05
445.3700
   CUFT/HR              4.0135+04  5184.0553    10.3442  3208.6323
10.3482
 STATE VARIABLES:
   TEMP   F               40.0000   372.1402    80.0000    10.0000
80.5645
   PRES   PSIA           300.0000   764.6959    15.0000    20.0000
35.0000
   VFRAC                  1.0000     0.0        0.0        0.0        0.0
   LFRAC                  0.0        1.0000     1.0000     1.0000
1.0000
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL            -415.9390 -5.6280+04 -1.1128+05 -1.8305+04 -
1.1124+05
   BTU/LB               -155.7275  -467.7049  -974.1294  -326.2555  -
973.8386
   BTU/HR              -9.3396+05 -8.3778+07 -4.3385+05 -4.1376+07 -
4.3372+05
 ENTROPY:
   BTU/LBMOL-R            -7.1490  -168.7933  -213.0830   -82.9510  -
213.0218
   BTU/LB-R               -2.6766    -1.4027    -1.8654    -1.4784    -
1.8648
 DENSITY:
   LBMOL/CUFT           5.5948-02     0.2871     0.3769     0.7044
0.3768
   LB/CUFT                0.1494    34.5533    43.0550    39.5246
43.0384
 AVG MW                   2.6709   120.3325   114.2309    56.1075
114.2309

 R1-FEED R1OUT R1RECIRC R2OUT R2RCYC2
```

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 STREAM ID               R1-FEED    R1OUT      R1RECIRC   R2OUT
R2RCYC2
 FROM :                  E-101      R-201      S1         R-401      E-
402
 TO   :                  M2         S1         P-201      C-401      M3

 SUBSTREAM: MIXED
 PHASE:                  MIXED      LIQUID     LIQUID     VAPOR
VAPOR
 COMPONENTS: LBMOL/HR
   ISOBUTYL            2279.3787   248.5975   206.5930   482.8003
440.7770
   ISOOCTAN             379.8792  2247.4297  1867.6913  4343.1031
3965.0765
   2:4:4-01              88.4093  4937.6152  4103.3280  1022.1653
933.1954
   TRIMERS             2.0273-06  1471.5426  1222.9025    57.1802
52.2032
   M-XYL-01               0.3408     2.0173     1.6764   428.7463
391.4280
   O-XYL-01               0.1312     0.7769     0.6457   426.3559
389.2456
   P-XYL-01               6.9968    41.4209    34.4222  7727.4282
7054.8277
   HYDROGEN               0.2260     1.3375     1.1115  2.5513+04
2.3292+04
 TOTAL FLOW:
   LBMOL/HR            2755.3620  8950.7376  7438.3707  4.0001+04
3.6519+04
   LB/HR               1.8200+05  1.0771+06  8.9514+05  1.6101+06
1.4700+06
   CUFT/HR             1.0734+04  3.1313+04  2.6022+04  1.7081+07
1.3148+07
 STATE VARIABLES:
   TEMP   F             347.0000   372.2713   372.2713  1000.5469
1050.0000
   PRES   PSIA          764.6959   764.6959   764.6959    36.6959
45.0000
   VFRAC               8.1361-02     0.0        0.0        1.0000
1.0000
   LFRAC                  0.9186     1.0000     1.0000     0.0        0.0
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL          -1.4632+04 -5.6938+04 -5.6938+04  1.3625+04
1.5239+04
   BTU/LB              -221.5205  -473.1353  -473.1353   338.4821
378.5701
   BTU/HR             -4.0316+07 -5.0963+08 -4.2352+08  5.4501+08
5.5650+08
 ENTROPY:
   BTU/LBMOL-R          -78.0842  -170.0445  -170.0445   -18.7736   -
18.0920
   BTU/LB-R              -1.1822    -1.4130    -1.4130    -0.4664    -
0.4495
 DENSITY:
   LBMOL/CUFT             0.2567     0.2858     0.2858  2.3418-03
2.7776-03
```

```
   LB/CUFT               16.9556    34.3991    34.3991  9.4263-02
0.1118
 AVG MW                  66.0525   120.3409   120.3409    40.2530
40.2530

 R2RECYCL R2TOXYLC REC1 REC2 RECGUESS
 ------------------------------------

 STREAM ID               R2RECYCL   R2TOXYLC   REC1       REC2
RECGUESS
 FROM :                  S2         S2         S-501      S-502      ----
 TO   :                  E-402      E-401      M-REC      M-REC      M1

 SUBSTREAM: MIXED
 PHASE:                  VAPOR      VAPOR      LIQUID     LIQUID
MIXED
 COMPONENTS: LBMOL/HR
   ISOBUTYL             440.7770    42.0233     3.7695    15.3061
19.0757
   ISOOCTAN            3965.0765   378.0266   296.7138    79.2666
375.9803
   2:4:4-01             933.1954    88.9699    71.0345    17.3748
88.4093
   TRIMERS               52.2032     4.9770  2.0244-06  2.9974-09
2.0273-06
   M-XYL-01             391.4280    37.3184     0.3239  1.6909-02
0.3408
   O-XYL-01             389.2456    37.1103     0.1260  5.2955-03
0.1312
   P-XYL-01            7054.8277   672.6004     6.6362     0.3610
6.9968
   HYDROGEN            2.3292+04  2220.6623  6.6475-02     0.1595
0.2260
 TOTAL FLOW:
   LBMOL/HR            3.6519+04  3481.6882   378.6703   112.4903
491.1600
   LB/HR               1.4700+06  1.4015+05  4.2829+04  1.1904+04
5.4733+04
   CUFT/HR             1.2905+07  1.2303+06  1000.5096   271.1485
1307.0350
 STATE VARIABLES:
   TEMP   F            1022.1082  1022.1082   100.0000    40.0000
86.0000
   PRES   PSIA           45.0000    45.0000    39.0000   300.0000
29.3959
   VFRAC                  1.0000     1.0000      0.0        0.0
3.7401-04
   LFRAC                  0.0        0.0         1.0000     1.0000
0.9996
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL           1.4325+04  1.4325+04 -9.8123+04 -9.2448+04 -
9.6893+04
   BTU/LB               355.8794   355.8794  -867.5494  -873.5947  -
869.4878
   BTU/HR              5.2314+08  4.9876+07 -3.7156+07 -1.0399+07 -
4.7590+07
 ENTROPY:
   BTU/LBMOL-R          -18.7027   -18.7027  -201.3060  -192.4343  -
199.2771
```

```
   BTU/LB-R              -0.4646    -0.4646    -1.7798    -1.8184     -
1.7883
 DENSITY:
   LBMOL/CUFT          2.8299-03  2.8299-03     0.3785     0.4149
0.3758
   LB/CUFT                0.1139     0.1139    42.8072    43.9029
41.8758
 AVG MW                  40.2530    40.2530   113.1036   105.8243
111.4364

 RECYCLE TO-F1 TO-H1 TO-M2 TO-P1
 -------------------------------

 STREAM ID               RECYCLE    TO-F1      TO-H1      TO-M2      TO-
P1
 FROM :                  M-REC      C-501      P-102      E-201      M1
 TO   :                  ----       S-502      E-101      M2         P-
102


 CONV. MAX. REL. ERR:     0.0        0.0        0.0      7.5408-05     0.0
 SUBSTREAM: MIXED
 PHASE:                  MIXED      VAPOR      LIQUID     LIQUID
MIXED
 COMPONENTS: LBMOL/HR
   ISOBUTYL              19.0757    38.2537  2279.3787   206.5958
2279.3787
   ISOOCTAN             375.9803    80.9830   379.8792  1867.5505
379.8792
   2:4:4-01              88.4093    17.7096    88.4093  4103.4136
88.4093
   TRIMERS             2.0274-06  2.9975-09  2.0273-06  1222.9451
2.0273-06
   M-XYL-01               0.3408  1.6959-02     0.3408     1.6765
0.3408
   O-XYL-01               0.1313  5.3075-03     0.1312     0.6457
0.1312
   P-XYL-01               6.9973     0.3621     6.9968    34.4242
6.9968
   HYDROGEN               0.2260  2220.5959     0.2260     1.1115
0.2260
 TOTAL FLOW:
   LBMOL/HR             491.1606  2357.9266  2755.3620  7438.3629
2755.3620
   LB/HR               5.4733+04  1.7902+04  1.8200+05  8.9514+05
1.8200+05
   CUFT/HR             1294.7945  7.7071+04  4542.7354  2.4057+04
4704.6610
 STATE VARIABLES:
   TEMP   F              87.1994   454.0701    39.3904   300.0000
30.8264
   PRES   PSIA           39.0000   300.0000   764.6959   784.6959
20.0000
   VFRAC               3.1460-04     1.0000     0.0        0.0
2.7307-04
   LFRAC                  0.9997     0.0        1.0000     1.0000
0.9997
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
```

```
   BTU/LBMOL          -9.6823+04  -227.4886 -3.2134+04 -6.3094+04 -
3.2446+04
   BTU/LB              -868.8642   -29.9638  -486.4917  -524.2932  -
491.2086
   BTU/HR             -4.7556+07 -5.3640+05 -8.8541+07 -4.6932+08 -
8.9399+07
 ENTROPY:
   BTU/LBMOL-R         -199.1508    -9.2201  -102.3393  -177.5194  -
102.9550
   BTU/LB-R              -1.7871    -1.2144    -1.5494    -1.4751    -
1.5587
 DENSITY:
   LBMOL/CUFT             0.3793 3.0594-02     0.6065     0.3092
0.5857
   LB/CUFT               42.2717     0.2323    40.0636    37.2085
38.6847
 AVG MW                 111.4364     7.5921    66.0525   120.3411
66.0525

 TO-R1 TO-R1HX TO-R2 TO-R2MIX TO-S2
 ----------------------------------

 STREAM ID                TO-R1      TO-R1HX    TO-R2      TO-R2MIX   TO-
S2
 FROM :                   M2         P-201      E-401      M3         C-
401
 TO   :                   R-201      E-201      M3         R-401      S2


 CONV. MAX. REL. ERR:      0.0        0.0        0.0    -7.3569-05     0.0
 SUBSTREAM: MIXED
 PHASE:                   LIQUID     LIQUID     VAPOR      VAPOR
VAPOR
 COMPONENTS: LBMOL/HR
   ISOBUTYL            2485.9745  206.5930    42.0044   482.8003
482.8003
   ISOOCTAN            2247.4297 1867.6913   377.9045  4343.1031
4343.1031
   2:4:4-01            4191.8229 4103.3280   829.2295  1762.3540
1022.1653
   TRIMERS             1222.9451 1222.9025     4.9728    57.1802
57.1802
   M-XYL-01               2.0173    1.6764     0.3148   391.7369
428.7463
   O-XYL-01               0.7769    0.6457     0.1163   389.3465
426.3559
   P-XYL-01              41.4209   34.4222     6.4745  7061.2583
7727.4282
   HYDROGEN               1.3375    1.1115     0.2260  2.3292+04
2.5513+04
 TOTAL FLOW:
   LBMOL/HR            1.0194+04 7438.3707  1261.2429  3.7780+04
4.0001+04
   LB/HR               1.0771+06 8.9514+05  1.4015+05  1.6101+06
1.6101+06
   CUFT/HR             3.0479+04 2.6028+04  2.5435+05  1.3454+07
1.4135+07
 STATE VARIABLES:
   TEMP   F             306.9507  372.4512   855.7711  1033.6018
1022.1082
```

```
   PRES   PSIA          764.6959   784.6959    70.0000    45.0000
45.0000
   VFRAC                  0.0        0.0        1.0000     1.0000
1.0000
   LFRAC                  1.0000     1.0000     0.0        0.0        0.0
   SFRAC                  0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL           -4.9995+04 -5.6921+04 -9092.3695  1.4426+04
1.4325+04
   BTU/LB                -473.1353  -473.0008   -81.8257   338.4821
355.8794
   BTU/HR              -5.0963+08 -4.2340+08 -1.1468+07  5.4501+08
5.7302+08
 ENTROPY:
   BTU/LBMOL-R          -149.7530  -170.0259  -113.0884   -21.0624   -
18.7027
   BTU/LB-R               -1.4172    -1.4129    -1.0177    -0.4942    -
0.4646
 DENSITY:
   LBMOL/CUFT             0.3345     0.2858  4.9587-03  2.8081-03
2.8299-03
   LB/CUFT               35.3409    34.3915     0.5510     0.1197
0.1139
 AVG MW                 105.6669   120.3409   111.1188    42.6189
40.2530

 TO-V1 TOTRCOL TOXYLCL TRIBOT TRIMERS
 ------------------------------------

 STREAM ID               TO-V1      TOTRCOL    TOXYLCL    TRIBOT
TRIMERS
 FROM :                  S1         V-301      E-401      S-301      E-
303
 TO   :                  V-301      S-301      S-501      E-303      ----

 SUBSTREAM: MIXED
 PHASE:                  LIQUID     MIXED      VAPOR      LIQUID
LIQUID
 COMPONENTS: LBMOL/HR
   ISOBUTYL               42.0044    42.0044    42.0233  3.5945-05
3.5945-05
   ISOOCTAN              379.7383   379.7383   378.0266     1.8338
1.8338
   2:4:4-01              834.2872   834.2872    88.9699     5.0577
5.0577
   TRIMERS               248.6401   248.6401     4.9770   243.6673
243.6673
   M-XYL-01                0.3409     0.3409    37.3184  2.6075-02
2.6075-02
   O-XYL-01                0.1313     0.1313    37.1103  1.4966-02
1.4966-02
   P-XYL-01                6.9987     6.9987   672.6004     0.5242
0.5242
   HYDROGEN                0.2260     0.2260  2220.6623  1.2875-15
1.2875-15
 TOTAL FLOW:
   LBMOL/HR             1512.3669  1512.3669  3481.6882   251.1240
251.1240
   LB/HR                1.8200+05  1.8200+05  1.4015+05  4.1852+04
4.1852+04
```

```
   CUFT/HR              5290.8242  3.0774+04  6.2209+05  1277.1560
891.3651
 STATE VARIABLES:
   TEMP   F              372.2713   355.3182   289.5669   543.0914
80.0000
   PRES   PSIA           764.6959    80.0000    45.0000    72.8400
60.0000
   VFRAC                   0.0        0.1594     1.0000     0.0        0.0
   LFRAC                   1.0000     0.8406     0.0        1.0000
1.0000
   SFRAC                   0.0        0.0        0.0        0.0        0.0
 ENTHALPY:
   BTU/LBMOL           -5.6938+04 -5.6938+04 -6029.7404 -4.6326+04 -
9.5273+04
   BTU/LB               -473.1353  -473.1353  -149.7961  -277.9713  -
571.6694
   BTU/HR              -8.6110+07 -8.6110+07 -2.0994+07 -1.1634+07 -
2.3925+07
 ENTROPY:
   BTU/LBMOL-R          -170.0445  -169.9281   -37.2400  -205.3884  -
268.5920
   BTU/LB-R               -1.4130    -1.4121    -0.9251    -1.2324    -
1.6116
 DENSITY:
   LBMOL/CUFT              0.2858  4.9144-02  5.5968-03     0.1966
0.2817
   LB/CUFT                34.3991     5.9140     0.2253    32.7695
46.9524
 AVG MW                  120.3409   120.3409    40.2530   166.6576
166.6576

 TRIOVHD XYLBOT XYLENE XYOVHD
 ----------------------------

 STREAM ID                TRIOVHD    XYLBOT     XYLENE     XYOVHD
 FROM :                   S-301      S-501      E-503      S-501
 TO   :                   E-401      E-503      ----       C-501

 SUBSTREAM: MIXED
 PHASE:                   LIQUID     LIQUID     LIQUID     VAPOR
 COMPONENTS: LBMOL/HR
   ISOBUTYL               42.0044  1.4468-15  1.4468-15    38.2537
   ISOOCTAN              377.9045     0.3298     0.3298    80.9830
   2:4:4-01              829.2295     0.2259     0.2259    17.7096
   TRIMERS                 4.9728     4.9770     4.9770  2.9975-09
   M-XYL-01                0.3148    36.9775    36.9775  1.6959-02
   O-XYL-01                0.1163    36.9790    36.9790  5.3075-03
   P-XYL-01                6.4745   665.6020   665.6020     0.3621
   HYDROGEN                0.2260  4.7032-22  4.7032-22  2220.5959
 TOTAL FLOW:
   LBMOL/HR             1261.2429   745.0912   745.0912  2357.9266
   LB/HR                1.4015+05  7.9418+04  7.9418+04  1.7902+04
   CUFT/HR              3630.0015  1814.0762  1482.3435  3.6312+05
 STATE VARIABLES:
   TEMP   F              239.5669   366.8821    80.0000   100.0000
   PRES   PSIA            70.0000    44.6800    35.0000    39.0000
   VFRAC                   0.0        0.0        0.0        1.0000
   LFRAC                   1.0000     1.0000     1.0000     0.0
   SFRAC                   0.0        0.0        0.0        0.0
 ENTHALPY:
```

```
  BTU/LBMOL          -6.5283+04  4160.6335 -1.0994+04 -3581.3276
  BTU/LB              -587.5032    39.0347  -103.1439  -471.7170
  BTU/HR             -8.2337+07  3.1001+06 -8.1915+06 -8.4445+06
ENTROPY:
  BTU/LBMOL-R         -172.6352   -85.9439  -107.8812    -9.7864
  BTU/LB-R              -1.5536    -0.8063    -1.0121    -1.2890
DENSITY:
  LBMOL/CUFT             0.3474     0.4107     0.5026  6.4935-03
  LB/CUFT               38.6082    43.7786    53.5758  4.9299-02
AVG MW                 111.1188   106.5880   106.5880     7.5921

EXHAUST
-------

STREAM ID               EXHAUST
FROM :                  S-502
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL              22.9476
  ISOOCTAN               1.7164
  2:4:4-01               0.3348
  TRIMERS             1.2065-13
  M-XYL-01            5.0184-05
  O-XYL-01            1.2027-05
  P-XYL-01            1.1265-03
  HYDROGEN            2220.4364
TOTAL FLOW:
  LBMOL/HR            2245.4364
  LB/HR               5997.4296
  CUFT/HR             4.0135+04
STATE VARIABLES:
  TEMP   F              40.0000
  PRES   PSIA          300.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL           -415.9390
  BTU/LB              -155.7275
  BTU/HR             -9.3396+05
ENTROPY:
  BTU/LBMOL-R           -7.1490
  BTU/LB-R              -2.6766
DENSITY:
  LBMOL/CUFT          5.5948-02
  LB/CUFT                0.1494
AVG MW                   2.6709

FDWU
----

STREAM ID               FDWU
FROM :                  ----
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  LIQUID
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL              41.1714
  ISOOCTAN             378.8524
  2:4:4-01             786.6263
  TRIMERS              246.8262
  M-XYL-01               1.6059
  O-XYL-01               0.6429
  P-XYL-01              32.8057
  HYDROGEN            6.2797-02
TOTAL FLOW:
  LBMOL/HR            1488.5937
  LB/HR               1.7913+05
  CUFT/HR             5184.0553
STATE VARIABLES:
  TEMP   F             372.1402
  PRES   PSIA          764.6959
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -5.6280+04
  BTU/LB              -467.7049
  BTU/HR             -8.3778+07
ENTROPY:
  BTU/LBMOL-R         -168.7933
  BTU/LB-R              -1.4027
DENSITY:
  LBMOL/CUFT             0.2871
  LB/CUFT               34.5533
AVG MW                 120.3325

I8--MAKE
--------

STREAM ID               I8--MAKE
FROM :                  ----
TO   :                  P-101

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL               0.0
  ISOOCTAN               3.8989
  2:4:4-01               0.0
  TRIMERS                0.0
  M-XYL-01               0.0
  O-XYL-01               0.0
  P-XYL-01               0.0
  HYDROGEN               0.0
TOTAL FLOW:
  LBMOL/HR               3.8989
  LB/HR                445.3700
  CUFT/HR               10.3442
STATE VARIABLES:
  TEMP   F              80.0000
  PRES   PSIA           15.0000
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
```

```
  BTU/LBMOL          -1.1128+05
  BTU/LB              -974.1294
  BTU/HR             -4.3385+05
ENTROPY:
  BTU/LBMOL-R         -213.0830
  BTU/LB-R              -1.8654
DENSITY:
  LBMOL/CUFT             0.3769
  LB/CUFT               43.0550
AVG MW                 114.2309

IBUTYLE
-------

STREAM ID               IBUTYLE
FROM :                  ----
TO   :                  M1

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            2260.3031
  ISOOCTAN                 0.0
  2:4:4-01                 0.0
  TRIMERS                  0.0
  M-XYL-01                 0.0
  O-XYL-01                 0.0
  P-XYL-01                 0.0
  HYDROGEN                 0.0
TOTAL FLOW:
  LBMOL/HR            2260.3031
  LB/HR               1.2682+05
  CUFT/HR             3208.6323
STATE VARIABLES:
  TEMP   F              10.0000
  PRES   PSIA           20.0000
  VFRAC                    0.0
  LFRAC                  1.0000
  SFRAC                    0.0
ENTHALPY:
  BTU/LBMOL          -1.8305+04
  BTU/LB              -326.2555
  BTU/HR             -4.1376+07
ENTROPY:
  BTU/LBMOL-R          -82.9510
  BTU/LB-R              -1.4784
DENSITY:
  LBMOL/CUFT             0.7044
  LB/CUFT               39.5246
AVG MW                  56.1075

ISOOCTAN
--------

STREAM ID               ISOOCTAN
FROM :                  P-101
TO   :                  M1

SUBSTREAM: MIXED
PHASE:                  LIQUID
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL               0.0
  ISOOCTAN               3.8989
  2:4:4-01               0.0
  TRIMERS                0.0
  M-XYL-01               0.0
  O-XYL-01               0.0
  P-XYL-01               0.0
  HYDROGEN               0.0
TOTAL FLOW:
  LBMOL/HR               3.8989
  LB/HR                445.3700
  CUFT/HR               10.3482
STATE VARIABLES:
  TEMP   F              80.5645
  PRES   PSIA           35.0000
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -1.1124+05
  BTU/LB               -973.8386
  BTU/HR             -4.3372+05
ENTROPY:
  BTU/LBMOL-R          -213.0218
  BTU/LB-R               -1.8648
DENSITY:
  LBMOL/CUFT             0.3768
  LB/CUFT               43.0384
AVG MW                 114.2309

R1-FEED
-------

STREAM ID               R1-FEED
FROM :                  E-101
TO   :                  M2

SUBSTREAM: MIXED
PHASE:                  MIXED
COMPONENTS: LBMOL/HR
  ISOBUTYL            2279.3787
  ISOOCTAN             379.8792
  2:4:4-01              88.4093
  TRIMERS             2.0273-06
  M-XYL-01               0.3408
  O-XYL-01               0.1312
  P-XYL-01               6.9968
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR            2755.3620
  LB/HR               1.8200+05
  CUFT/HR             1.0734+04
STATE VARIABLES:
  TEMP   F             347.0000
  PRES   PSIA          764.6959
  VFRAC               8.1361-02
  LFRAC                  0.9186
  SFRAC                  0.0
ENTHALPY:
```

```
  BTU/LBMOL          -1.4632+04
  BTU/LB              -221.5205
  BTU/HR             -4.0316+07
ENTROPY:
  BTU/LBMOL-R          -78.0842
  BTU/LB-R              -1.1822
DENSITY:
  LBMOL/CUFT             0.2567
  LB/CUFT               16.9556
AVG MW                  66.0525

R1OUT
-----

STREAM ID               R1OUT
FROM :                  R-201
TO   :                  S1

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL             248.5975
  ISOOCTAN            2247.4297
  2:4:4-01            4937.6152
  TRIMERS             1471.5426
  M-XYL-01               2.0173
  O-XYL-01               0.7769
  P-XYL-01              41.4209
  HYDROGEN               1.3375
TOTAL FLOW:
  LBMOL/HR            8950.7376
  LB/HR               1.0771+06
  CUFT/HR             3.1313+04
STATE VARIABLES:
  TEMP   F             372.2713
  PRES   PSIA          764.6959
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -5.6938+04
  BTU/LB              -473.1353
  BTU/HR             -5.0963+08
ENTROPY:
  BTU/LBMOL-R         -170.0445
  BTU/LB-R              -1.4130
DENSITY:
  LBMOL/CUFT             0.2858
  LB/CUFT               34.3991
AVG MW                 120.3409

R1RECIRC
--------

STREAM ID               R1RECIRC
FROM :                  S1
TO   :                  P-201

SUBSTREAM: MIXED
PHASE:                  LIQUID
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL            206.5930
  ISOOCTAN           1867.6913
  2:4:4-01           4103.3280
  TRIMERS            1222.9025
  M-XYL-01              1.6764
  O-XYL-01              0.6457
  P-XYL-01             34.4222
  HYDROGEN              1.1115
TOTAL FLOW:
  LBMOL/HR           7438.3707
  LB/HR              8.9514+05
  CUFT/HR            2.6022+04
STATE VARIABLES:
  TEMP   F            372.2713
  PRES   PSIA         764.6959
  VFRAC                 0.0
  LFRAC                 1.0000
  SFRAC                 0.0
ENTHALPY:
  BTU/LBMOL         -5.6938+04
  BTU/LB             -473.1353
  BTU/HR            -4.2352+08
ENTROPY:
  BTU/LBMOL-R        -170.0445
  BTU/LB-R             -1.4130
DENSITY:
  LBMOL/CUFT            0.2858
  LB/CUFT              34.3991
AVG MW                120.3409

R2OUT
-----

STREAM ID               R2OUT
FROM :                  R-401
TO   :                  C-401

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL            482.8003
  ISOOCTAN           4343.1031
  2:4:4-01           1022.1653
  TRIMERS              57.1802
  M-XYL-01            428.7463
  O-XYL-01            426.3559
  P-XYL-01           7727.4282
  HYDROGEN           2.5513+04
TOTAL FLOW:
  LBMOL/HR           4.0001+04
  LB/HR              1.6101+06
  CUFT/HR            1.7081+07
STATE VARIABLES:
  TEMP   F           1000.5469
  PRES   PSIA          36.6959
  VFRAC                 1.0000
  LFRAC                 0.0
  SFRAC                 0.0
ENTHALPY:
```

```
  BTU/LBMOL           1.3625+04
  BTU/LB               338.4821
  BTU/HR              5.4501+08
ENTROPY:
  BTU/LBMOL-R          -18.7736
  BTU/LB-R              -0.4664
DENSITY:
  LBMOL/CUFT          2.3418-03
  LB/CUFT             9.4263-02
AVG MW                  40.2530

R2RCYC2
-------

STREAM ID               R2RCYC2
FROM :                  E-402
TO   :                  M3

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL             440.7770
  ISOOCTAN            3965.0765
  2:4:4-01             933.1954
  TRIMERS               52.2032
  M-XYL-01             391.4280
  O-XYL-01             389.2456
  P-XYL-01            7054.8277
  HYDROGEN            2.3292+04
TOTAL FLOW:
  LBMOL/HR            3.6519+04
  LB/HR               1.4700+06
  CUFT/HR             1.3148+07
STATE VARIABLES:
  TEMP   F            1050.0000
  PRES   PSIA           45.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL           1.5239+04
  BTU/LB               378.5701
  BTU/HR              5.5650+08
ENTROPY:
  BTU/LBMOL-R          -18.0920
  BTU/LB-R              -0.4495
DENSITY:
  LBMOL/CUFT          2.7776-03
  LB/CUFT                0.1118
AVG MW                  40.2530

R2RECYCL
--------

STREAM ID               R2RECYCL
FROM :                  S2
TO   :                  E-402

SUBSTREAM: MIXED
PHASE:                  VAPOR
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL             440.7770
  ISOOCTAN            3965.0765
  2:4:4-01             933.1954
  TRIMERS               52.2032
  M-XYL-01             391.4280
  O-XYL-01             389.2456
  P-XYL-01            7054.8277
  HYDROGEN            2.3292+04
TOTAL FLOW:
  LBMOL/HR            3.6519+04
  LB/HR               1.4700+06
  CUFT/HR             1.2905+07
STATE VARIABLES:
  TEMP   F            1022.1082
  PRES   PSIA           45.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL           1.4325+04
  BTU/LB               355.8794
  BTU/HR              5.2314+08
ENTROPY:
  BTU/LBMOL-R          -18.7027
  BTU/LB-R              -0.4646
DENSITY:
  LBMOL/CUFT          2.8299-03
  LB/CUFT                0.1139
AVG MW                  40.2530

R2TOXYLC
--------

STREAM ID               R2TOXYLC
FROM :                  S2
TO   :                  E-401

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL              42.0233
  ISOOCTAN             378.0266
  2:4:4-01              88.9699
  TRIMERS                4.9770
  M-XYL-01              37.3184
  O-XYL-01              37.1103
  P-XYL-01             672.6004
  HYDROGEN            2220.6623
TOTAL FLOW:
  LBMOL/HR            3481.6882
  LB/HR               1.4015+05
  CUFT/HR             1.2303+06
STATE VARIABLES:
  TEMP   F            1022.1082
  PRES   PSIA           45.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
```

```
  BTU/LBMOL           1.4325+04
  BTU/LB               355.8794
  BTU/HR              4.9876+07
ENTROPY:
  BTU/LBMOL-R          -18.7027
  BTU/LB-R              -0.4646
DENSITY:
  LBMOL/CUFT          2.8299-03
  LB/CUFT                0.1139
AVG MW                  40.2530

REC1
----

STREAM ID               REC1
FROM :                  S-501
TO   :                  M-REC

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL               3.7695
  ISOOCTAN             296.7138
  2:4:4-01              71.0345
  TRIMERS             2.0244-06
  M-XYL-01               0.3239
  O-XYL-01               0.1260
  P-XYL-01               6.6362
  HYDROGEN            6.6475-02
TOTAL FLOW:
  LBMOL/HR             378.6703
  LB/HR               4.2829+04
  CUFT/HR             1000.5096
STATE VARIABLES:
  TEMP   F             100.0000
  PRES   PSIA           39.0000
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -9.8123+04
  BTU/LB              -867.5494
  BTU/HR             -3.7156+07
ENTROPY:
  BTU/LBMOL-R         -201.3060
  BTU/LB-R              -1.7798
DENSITY:
  LBMOL/CUFT             0.3785
  LB/CUFT               42.8072
AVG MW                 113.1036

REC2
----

STREAM ID               REC2
FROM :                  S-502
TO   :                  M-REC

SUBSTREAM: MIXED
PHASE:                  LIQUID
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL              15.3061
  ISOOCTAN              79.2666
  2:4:4-01              17.3748
  TRIMERS             2.9974-09
  M-XYL-01            1.6909-02
  O-XYL-01            5.2955-03
  P-XYL-01               0.3610
  HYDROGEN               0.1595
TOTAL FLOW:
  LBMOL/HR             112.4903
  LB/HR               1.1904+04
  CUFT/HR              271.1485
STATE VARIABLES:
  TEMP   F              40.0000
  PRES   PSIA          300.0000
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -9.2448+04
  BTU/LB              -873.5947
  BTU/HR             -1.0399+07
ENTROPY:
  BTU/LBMOL-R         -192.4343
  BTU/LB-R              -1.8184
DENSITY:
  LBMOL/CUFT             0.4149
  LB/CUFT               43.9029
AVG MW                 105.8243

RECGUESS
--------

STREAM ID               RECGUESS
FROM :                  ----
TO   :                  M1

SUBSTREAM: MIXED
PHASE:                  MIXED
COMPONENTS: LBMOL/HR
  ISOBUTYL              19.0757
  ISOOCTAN             375.9803
  2:4:4-01              88.4093
  TRIMERS             2.0273-06
  M-XYL-01               0.3408
  O-XYL-01               0.1312
  P-XYL-01               6.9968
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR             491.1600
  LB/HR               5.4733+04
  CUFT/HR             1307.0350
STATE VARIABLES:
  TEMP   F              86.0000
  PRES   PSIA           29.3959
  VFRAC               3.7401-04
  LFRAC                  0.9996
  SFRAC                  0.0
ENTHALPY:
```

```
  BTU/LBMOL          -9.6893+04
  BTU/LB              -869.4878
  BTU/HR             -4.7590+07
ENTROPY:
  BTU/LBMOL-R         -199.2771
  BTU/LB-R              -1.7883
DENSITY:
  LBMOL/CUFT             0.3758
  LB/CUFT               41.8758
AVG MW                 111.4364

RECYCLE
-------

STREAM ID               RECYCLE
FROM :                  M-REC
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  MIXED
COMPONENTS: LBMOL/HR
  ISOBUTYL              19.0757
  ISOOCTAN             375.9803
  2:4:4-01              88.4093
  TRIMERS             2.0274-06
  M-XYL-01               0.3408
  O-XYL-01               0.1313
  P-XYL-01               6.9973
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR             491.1606
  LB/HR               5.4733+04
  CUFT/HR             1294.7945
STATE VARIABLES:
  TEMP   F              87.1994
  PRES   PSIA           39.0000
  VFRAC               3.1460-04
  LFRAC                  0.9997
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -9.6823+04
  BTU/LB              -868.8642
  BTU/HR             -4.7556+07
ENTROPY:
  BTU/LBMOL-R         -199.1508
  BTU/LB-R              -1.7871
DENSITY:
  LBMOL/CUFT             0.3793
  LB/CUFT               42.2717
AVG MW                 111.4364

TO-F1
-----

STREAM ID               TO-F1
FROM :                  C-501
TO   :                  S-502

SUBSTREAM: MIXED
PHASE:                  VAPOR
```

```
COMPONENTS: LBMOL/HR
  ISOBUTYL              38.2537
  ISOOCTAN              80.9830
  2:4:4-01              17.7096
  TRIMERS             2.9975-09
  M-XYL-01            1.6959-02
  O-XYL-01            5.3075-03
  P-XYL-01               0.3621
  HYDROGEN            2220.5959
TOTAL FLOW:
  LBMOL/HR            2357.9266
  LB/HR               1.7902+04
  CUFT/HR             7.7071+04
STATE VARIABLES:
  TEMP   F             454.0701
  PRES   PSIA          300.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL           -227.4886
  BTU/LB               -29.9638
  BTU/HR             -5.3640+05
ENTROPY:
  BTU/LBMOL-R           -9.2201
  BTU/LB-R              -1.2144
DENSITY:
  LBMOL/CUFT          3.0594-02
  LB/CUFT                0.2323
AVG MW                   7.5921

TO-H1
-----

STREAM ID               TO-H1
FROM :                  P-102
TO   :                  E-101

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            2279.3787
  ISOOCTAN             379.8792
  2:4:4-01              88.4093
  TRIMERS             2.0273-06
  M-XYL-01               0.3408
  O-XYL-01               0.1312
  P-XYL-01               6.9968
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR            2755.3620
  LB/HR               1.8200+05
  CUFT/HR             4542.7354
STATE VARIABLES:
  TEMP   F              39.3904
  PRES   PSIA          764.6959
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
```

```
  BTU/LBMOL          -3.2134+04
  BTU/LB              -486.4917
  BTU/HR             -8.8541+07
ENTROPY:
  BTU/LBMOL-R         -102.3393
  BTU/LB-R              -1.5494
DENSITY:
  LBMOL/CUFT             0.6065
  LB/CUFT               40.0636
AVG MW                  66.0525

TO-M2
-----

STREAM ID               TO-M2
FROM :                  E-201
TO   :                  M2


CONV. MAX. REL. ERR:  7.5408-05
SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL             206.5958
  ISOOCTAN            1867.5505
  2:4:4-01            4103.4136
  TRIMERS             1222.9451
  M-XYL-01               1.6765
  O-XYL-01               0.6457
  P-XYL-01              34.4242
  HYDROGEN               1.1115
TOTAL FLOW:
  LBMOL/HR            7438.3629
  LB/HR              8.9514+05
  CUFT/HR            2.4057+04
STATE VARIABLES:
  TEMP   F             300.0000
  PRES   PSIA          784.6959
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -6.3094+04
  BTU/LB              -524.2932
  BTU/HR             -4.6932+08
ENTROPY:
  BTU/LBMOL-R         -177.5194
  BTU/LB-R              -1.4751
DENSITY:
  LBMOL/CUFT             0.3092
  LB/CUFT               37.2085
AVG MW                 120.3411

TO-P1
-----

STREAM ID               TO-P1
FROM :                  M1
TO   :                  P-102
```

```
SUBSTREAM: MIXED
PHASE:                  MIXED
COMPONENTS: LBMOL/HR
  ISOBUTYL            2279.3787
  ISOOCTAN             379.8792
  2:4:4-01              88.4093
  TRIMERS             2.0273-06
  M-XYL-01               0.3408
  O-XYL-01               0.1312
  P-XYL-01               6.9968
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR            2755.3620
  LB/HR               1.8200+05
  CUFT/HR             4704.6610
STATE VARIABLES:
  TEMP   F              30.8264
  PRES   PSIA           20.0000
  VFRAC               2.7307-04
  LFRAC                  0.9997
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -3.2446+04
  BTU/LB              -491.2086
  BTU/HR             -8.9399+07
ENTROPY:
  BTU/LBMOL-R         -102.9550
  BTU/LB-R              -1.5587
DENSITY:
  LBMOL/CUFT             0.5857
  LB/CUFT               38.6847
AVG MW                  66.0525

TO-R1
-----

STREAM ID               TO-R1
FROM :                  M2
TO   :                  R-201

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            2485.9745
  ISOOCTAN            2247.4297
  2:4:4-01            4191.8229
  TRIMERS             1222.9451
  M-XYL-01               2.0173
  O-XYL-01               0.7769
  P-XYL-01              41.4209
  HYDROGEN               1.3375
TOTAL FLOW:
  LBMOL/HR            1.0194+04
  LB/HR               1.0771+06
  CUFT/HR             3.0479+04
STATE VARIABLES:
  TEMP   F             306.9507
  PRES   PSIA          764.6959
  VFRAC                  0.0
  LFRAC                  1.0000
```

```
  SFRAC                    0.0
ENTHALPY:
  BTU/LBMOL            -4.9995+04
  BTU/LB               -473.1353
  BTU/HR               -5.0963+08
ENTROPY:
  BTU/LBMOL-R          -149.7530
  BTU/LB-R               -1.4172
DENSITY:
  LBMOL/CUFT              0.3345
  LB/CUFT                35.3409
AVG MW                  105.6669

TO-R1HX
-------

STREAM ID               TO-R1HX
FROM :                  P-201
TO   :                  E-201

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL              206.5930
  ISOOCTAN             1867.6913
  2:4:4-01             4103.3280
  TRIMERS              1222.9025
  M-XYL-01                1.6764
  O-XYL-01                0.6457
  P-XYL-01               34.4222
  HYDROGEN                1.1115
TOTAL FLOW:
  LBMOL/HR             7438.3707
  LB/HR                8.9514+05
  CUFT/HR              2.6028+04
STATE VARIABLES:
  TEMP   F              372.4512
  PRES   PSIA           784.6959
  VFRAC                   0.0
  LFRAC                   1.0000
  SFRAC                   0.0
ENTHALPY:
  BTU/LBMOL            -5.6921+04
  BTU/LB               -473.0008
  BTU/HR               -4.2340+08
ENTROPY:
  BTU/LBMOL-R          -170.0259
  BTU/LB-R               -1.4129
DENSITY:
  LBMOL/CUFT              0.2858
  LB/CUFT                34.3915
AVG MW                  120.3409

TO-R2
-----

STREAM ID               TO-R2
FROM :                  E-401
TO   :                  M3
```

```
SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL               42.0044
  ISOOCTAN              377.9045
  2:4:4-01              829.2295
  TRIMERS                 4.9728
  M-XYL-01                0.3148
  O-XYL-01                0.1163
  P-XYL-01                6.4745
  HYDROGEN                0.2260
TOTAL FLOW:
  LBMOL/HR             1261.2429
  LB/HR                1.4015+05
  CUFT/HR              2.5435+05
STATE VARIABLES:
  TEMP   F              855.7711
  PRES   PSIA            70.0000
  VFRAC                   1.0000
  LFRAC                   0.0
  SFRAC                   0.0
ENTHALPY:
  BTU/LBMOL           -9092.3695
  BTU/LB                -81.8257
  BTU/HR              -1.1468+07
ENTROPY:
  BTU/LBMOL-R          -113.0884
  BTU/LB-R               -1.0177
DENSITY:
  LBMOL/CUFT           4.9587-03
  LB/CUFT                 0.5510
AVG MW                  111.1188

TO-R2MIX
--------

STREAM ID               TO-R2MIX
FROM :                  M3
TO   :                  R-401


CONV. MAX. REL. ERR: -7.3569-05
SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL              482.8003
  ISOOCTAN             4343.1031
  2:4:4-01             1762.3540
  TRIMERS                57.1802
  M-XYL-01              391.7369
  O-XYL-01              389.3465
  P-XYL-01             7061.2583
  HYDROGEN             2.3292+04
TOTAL FLOW:
  LBMOL/HR             3.7780+04
  LB/HR                1.6101+06
  CUFT/HR              1.3454+07
STATE VARIABLES:
  TEMP   F             1033.6018
  PRES   PSIA            45.0000
```

```
  VFRAC                   1.0000
  LFRAC                   0.0
  SFRAC                   0.0
ENTHALPY:
  BTU/LBMOL             1.4426+04
  BTU/LB                 338.4821
  BTU/HR                5.4501+08
ENTROPY:
  BTU/LBMOL-R            -21.0624
  BTU/LB-R                -0.4942
DENSITY:
  LBMOL/CUFT            2.8081-03
  LB/CUFT                 0.1197
AVG MW                   42.6189

TO-S2
-----

STREAM ID                TO-S2
FROM :                   C-401
TO   :                   S2

SUBSTREAM: MIXED
PHASE:                   VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL               482.8003
  ISOOCTAN              4343.1031
  2:4:4-01              1022.1653
  TRIMERS                 57.1802
  M-XYL-01               428.7463
  O-XYL-01               426.3559
  P-XYL-01              7727.4282
  HYDROGEN              2.5513+04
TOTAL FLOW:
  LBMOL/HR              4.0001+04
  LB/HR                 1.6101+06
  CUFT/HR               1.4135+07
STATE VARIABLES:
  TEMP   F              1022.1082
  PRES   PSIA             45.0000
  VFRAC                   1.0000
  LFRAC                   0.0
  SFRAC                   0.0
ENTHALPY:
  BTU/LBMOL             1.4325+04
  BTU/LB                 355.8794
  BTU/HR                5.7302+08
ENTROPY:
  BTU/LBMOL-R            -18.7027
  BTU/LB-R                -0.4646
DENSITY:
  LBMOL/CUFT            2.8299-03
  LB/CUFT                 0.1139
AVG MW                   40.2530

TO-V1
-----

STREAM ID                TO-V1
FROM :                   S1
```

```
TO   :                  V-301

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL               42.0044
  ISOOCTAN              379.7383
  2:4:4-01              834.2872
  TRIMERS               248.6401
  M-XYL-01                0.3409
  O-XYL-01                0.1313
  P-XYL-01                6.9987
  HYDROGEN                0.2260
TOTAL FLOW:
  LBMOL/HR             1512.3669
  LB/HR                1.8200+05
  CUFT/HR              5290.8242
STATE VARIABLES:
  TEMP   F              372.2713
  PRES   PSIA           764.6959
  VFRAC                   0.0
  LFRAC                   1.0000
  SFRAC                   0.0
ENTHALPY:
  BTU/LBMOL           -5.6938+04
  BTU/LB               -473.1353
  BTU/HR              -8.6110+07
ENTROPY:
  BTU/LBMOL-R          -170.0445
  BTU/LB-R               -1.4130
DENSITY:
  LBMOL/CUFT              0.2858
  LB/CUFT                34.3991
AVG MW                  120.3409

TOTRCOL
-------

STREAM ID               TOTRCOL
FROM :                  V-301
TO   :                  S-301

SUBSTREAM: MIXED
PHASE:                  MIXED
COMPONENTS: LBMOL/HR
  ISOBUTYL               42.0044
  ISOOCTAN              379.7383
  2:4:4-01              834.2872
  TRIMERS               248.6401
  M-XYL-01                0.3409
  O-XYL-01                0.1313
  P-XYL-01                6.9987
  HYDROGEN                0.2260
TOTAL FLOW:
  LBMOL/HR             1512.3669
  LB/HR                1.8200+05
  CUFT/HR              3.0774+04
STATE VARIABLES:
  TEMP   F              355.3182
  PRES   PSIA            80.0000
```

```
  VFRAC                  0.1594
  LFRAC                  0.8406
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -5.6938+04
  BTU/LB              -473.1353
  BTU/HR             -8.6110+07
ENTROPY:
  BTU/LBMOL-R         -169.9281
  BTU/LB-R              -1.4121
DENSITY:
  LBMOL/CUFT          4.9144-02
  LB/CUFT                5.9140
AVG MW                 120.3409

TOXYLCL
-------

STREAM ID               TOXYLCL
FROM :                  E-401
TO   :                  S-501

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL              42.0233
  ISOOCTAN             378.0266
  2:4:4-01              88.9699
  TRIMERS                4.9770
  M-XYL-01              37.3184
  O-XYL-01              37.1103
  P-XYL-01             672.6004
  HYDROGEN            2220.6623
TOTAL FLOW:
  LBMOL/HR            3481.6882
  LB/HR               1.4015+05
  CUFT/HR             6.2209+05
STATE VARIABLES:
  TEMP   F             289.5669
  PRES   PSIA           45.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -6029.7404
  BTU/LB              -149.7961
  BTU/HR             -2.0994+07
ENTROPY:
  BTU/LBMOL-R          -37.2400
  BTU/LB-R              -0.9251
DENSITY:
  LBMOL/CUFT          5.5968-03
  LB/CUFT                0.2253
AVG MW                  40.2530

TRIBOT
------

STREAM ID               TRIBOT
FROM :                  S-301
```

```
TO   :                  E-303

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            3.5945-05
  ISOOCTAN               1.8338
  2:4:4-01               5.0577
  TRIMERS              243.6673
  M-XYL-01            2.6075-02
  O-XYL-01            1.4966-02
  P-XYL-01               0.5242
  HYDROGEN            1.2875-15
TOTAL FLOW:
  LBMOL/HR             251.1240
  LB/HR               4.1852+04
  CUFT/HR             1277.1560
STATE VARIABLES:
  TEMP   F             543.0914
  PRES   PSIA           72.8400
  VFRAC                 0.0
  LFRAC                  1.0000
  SFRAC                 0.0
ENTHALPY:
  BTU/LBMOL          -4.6326+04
  BTU/LB              -277.9713
  BTU/HR             -1.1634+07
ENTROPY:
  BTU/LBMOL-R         -205.3884
  BTU/LB-R              -1.2324
DENSITY:
  LBMOL/CUFT             0.1966
  LB/CUFT               32.7695
AVG MW                 166.6576

TRIMERS
-------

STREAM ID               TRIMERS
FROM :                  E-303
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            3.5945-05
  ISOOCTAN               1.8338
  2:4:4-01               5.0577
  TRIMERS              243.6673
  M-XYL-01            2.6075-02
  O-XYL-01            1.4966-02
  P-XYL-01               0.5242
  HYDROGEN            1.2875-15
TOTAL FLOW:
  LBMOL/HR             251.1240
  LB/HR               4.1852+04
  CUFT/HR              891.3651
STATE VARIABLES:
  TEMP   F              80.0000
  PRES   PSIA           60.0000
```

```
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -9.5273+04
  BTU/LB              -571.6694
  BTU/HR             -2.3925+07
ENTROPY:
  BTU/LBMOL-R         -268.5920
  BTU/LB-R              -1.6116
DENSITY:
  LBMOL/CUFT             0.2817
  LB/CUFT               46.9524
AVG MW                 166.6576

TRIOVHD
-------

STREAM ID               TRIOVHD
FROM :                  S-301
TO   :                  E-401

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL              42.0044
  ISOOCTAN             377.9045
  2:4:4-01             829.2295
  TRIMERS                4.9728
  M-XYL-01               0.3148
  O-XYL-01               0.1163
  P-XYL-01               6.4745
  HYDROGEN               0.2260
TOTAL FLOW:
  LBMOL/HR            1261.2429
  LB/HR               1.4015+05
  CUFT/HR             3630.0015
STATE VARIABLES:
  TEMP   F             239.5669
  PRES   PSIA           70.0000
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -6.5283+04
  BTU/LB              -587.5032
  BTU/HR             -8.2337+07
ENTROPY:
  BTU/LBMOL-R         -172.6352
  BTU/LB-R              -1.5536
DENSITY:
  LBMOL/CUFT             0.3474
  LB/CUFT               38.6082
AVG MW                 111.1188

XYLBOT
------

STREAM ID               XYLBOT
FROM :                  S-501
```

```
TO   :                  E-503

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            1.4468-15
  ISOOCTAN               0.3298
  2:4:4-01               0.2259
  TRIMERS                4.9770
  M-XYL-01              36.9775
  O-XYL-01              36.9790
  P-XYL-01             665.6020
  HYDROGEN            4.7032-22
TOTAL FLOW:
  LBMOL/HR             745.0912
  LB/HR               7.9418+04
  CUFT/HR             1814.0762
STATE VARIABLES:
  TEMP   F             366.8821
  PRES   PSIA           44.6800
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL           4160.6335
  BTU/LB                39.0347
  BTU/HR              3.1001+06
ENTROPY:
  BTU/LBMOL-R          -85.9439
  BTU/LB-R              -0.8063
DENSITY:
  LBMOL/CUFT             0.4107
  LB/CUFT               43.7786
AVG MW                 106.5880

XYLENE
------

STREAM ID               XYLENE
FROM :                  E-503
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: LBMOL/HR
  ISOBUTYL            1.4468-15
  ISOOCTAN               0.3298
  2:4:4-01               0.2259
  TRIMERS                4.9770
  M-XYL-01              36.9775
  O-XYL-01              36.9790
  P-XYL-01             665.6020
  HYDROGEN            4.7032-22
TOTAL FLOW:
  LBMOL/HR             745.0912
  LB/HR               7.9418+04
  CUFT/HR             1482.3435
STATE VARIABLES:
  TEMP   F              80.0000
  PRES   PSIA           35.0000
```

```
  VFRAC                  0.0
  LFRAC                  1.0000
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -1.0994+04
  BTU/LB              -103.1439
  BTU/HR             -8.1915+06
ENTROPY:
  BTU/LBMOL-R         -107.8812
  BTU/LB-R              -1.0121
DENSITY:
  LBMOL/CUFT             0.5026
  LB/CUFT               53.5758
AVG MW                 106.5880

XYOVHD
------

STREAM ID               XYOVHD
FROM :                  S-501
TO   :                  C-501

SUBSTREAM: MIXED
PHASE:                  VAPOR
COMPONENTS: LBMOL/HR
  ISOBUTYL              38.2537
  ISOOCTAN              80.9830
  2:4:4-01              17.7096
  TRIMERS             2.9975-09
  M-XYL-01            1.6959-02
  O-XYL-01            5.3075-03
  P-XYL-01               0.3621
  HYDROGEN            2220.5959
TOTAL FLOW:
  LBMOL/HR            2357.9266
  LB/HR               1.7902+04
  CUFT/HR             3.6312+05
STATE VARIABLES:
  TEMP   F             100.0000
  PRES   PSIA           39.0000
  VFRAC                  1.0000
  LFRAC                  0.0
  SFRAC                  0.0
ENTHALPY:
  BTU/LBMOL          -3581.3276
  BTU/LB              -471.7170
  BTU/HR             -8.4445+06
ENTROPY:
  BTU/LBMOL-R           -9.7864
  BTU/LB-R              -1.2890
DENSITY:
  LBMOL/CUFT          6.4935-03
  LB/CUFT             4.9299-02
AVG MW                   7.5921
```