Fluidized Catalytic Cracking to Convert Biomass to Fuels

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Fluidized Catalytic Cracking to Convert Biomass to Fuels

**Abstract**
The process of biomass fluidized catalytic cracking (BFCC) has been adapted from the traditional fluidized catalytic cracking of crude oil in petroleum refineries. Instead of a naphtha feedstock, BFCC can accommodate various types of biomass that is cracked into more valuable aromatic and olefinic compounds. This plant inputs forest biomass and will be located in southwestern Louisiana, where wood output exceeds 100 million kg/yr in over ten counties. Biomass, procured in the form of wood chips, must first be dried to a moisture content below 10 wt% and crushed to a particle size of 100-500 micron. The wood sawdust is then fed to a circulating fluidized bed riser, where it undergoes catalytic fast pyrolysis (CFP) in the presence of a ZSM-5 catalyst. CFP occurs at a high temperature of 600 °C, producing an effluent syngas composed of aromatics, olefins, and volatiles. The biogas is separated from water and volatiles, produced by deoxygenation processes, in a three phase pressure vessel. The more valuable products of benzene, toluene, and xylenes are then separated from the high-boiling components. The proposed design converts 400,000 metric tons of wood to 17.4 million kilograms of a BTX mixture per year, including 4.6, 7, and 3.3 million kilograms per year of benzene, toluene, and xylenes, respectively. In addition, 345 GWh of electricity is produced yearly as a byproduct. The required total permanent investment for this project is $93 MM. At a discount rate of 10% and BTX sale price of $1.1/kg, the base case net present value (NPV) is $(157 MM) and the expected ROI is -20%. The result of this base case analysis suggests that this project should not be further pursued. The best case scenario assumed double the yield of BTX at a sale price of $1.54/kg and a renewable fuel credit of $1.01/gal, resulting in a NPV of $506 MM, an IRR of 70%, and a ROI of 81 %. The economic feasibility of this project is also sensitive to the availability and price of biomass, as well as the catalyst degeneration rate within the system.

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

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Dear Prof. Fabiano, Dr. Sinno and Dr. Targett,

Enclosed is our completed proposal for the project “Fluidized Catalytic Cracking to Convert Biomass to Fuels,” as proposed by Dr. Matthew Targett of LP Amina, in fulfillment of the requirements of CBE 459. The proposed design applies catalytic fast pyrolysis (CFP) to wood chips in a circulating fluidized bed riser in the presence of a ZSM-5 catalyst. The CFP products include volatile gases, coke, and a mixture of aromatics. The aromatic products are separated from the coke and volatiles to yield BTX. The heat network of the process has been optimized to produce steam for electricity generation. This process is renewable and utilizes non-food source biomass available in excess in the U.S.

Although the market for BTX is currently in decline, the global petrochemicals market was valued at $559 billion in 2013 and is predicted to grow to $885 billion by 2020. BTX represents a $120 billion global market, historically growing at rates greater than the global GDP. BTX and its derivatives comprise feedstocks used by the chemical industry to make products such as automobile tires, nylon, laundry detergent, polyester clothing and packaging.

The proposed design converts 400,000 metric tons of dry wood biomass to approximately 17.4 million kilograms of a BTX mixture per year, including 4.6, 7, and 3.3 million kilograms per year of benzene, toluene, and xylenes, respectively. In addition, almost 345 GWh/yr of electricity is produced.

The required total permanent investment for this project is $93 MM. At a discount rate of 10% and a BTX sale price of $1.1/kg, the base case NPV is $(157 MM) and the projected ROI is -20%. The best case scenario assumed double the yield of BTX at a sale price of $1.54/kg and a renewable fuel credit of $1.01/gal, resulting in a NPV of $506 MM, an IRR of 70%, and a ROI of 86%. The result of this base case analysis suggests that this project should not be pursued further.

Sincerely,

Stephen Boust  Mo Green  Serena Machi
FLUIDIZED CATALYTIC CRACKING TO CONVERT BIOMASS TO FUELS

Stephen Boust
Mo Green
Serena Machi

April 14, 2015

Industrial Consultant:
Dr. Matthew Targett, LP Amina

Faculty Advisor:
Dr. Talid Sinno, University of Pennsylvania

Department of Chemical and Biomolecular Engineering
School of Engineering and Applied Science
University of Pennsylvania
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1. ABSTRACT
The process of biomass fluidized catalytic cracking (BFCC) has been adapted from the traditional fluidized catalytic cracking of crude oil in petroleum refineries. Instead of a naphtha feedstock, BFCC can accommodate various types of biomass that is cracked into more valuable aromatic and olefinic compounds. This plant inputs forest biomass and will be located in southwestern Louisiana, where wood output exceeds 100 million kg/yr in over ten counties.

Biomass, procured in the form of wood chips, must first be dried to a moisture content below 10 wt% and crushed to a particle size of 100-500 micron. The wood sawdust is then fed to a circulating fluidized bed riser, where it undergoes catalytic fast pyrolysis (CFP) in the presence of a ZSM-5 catalyst. CFP occurs at a high temperature of 600 °C, producing an effluent syngas composed of aromatics, olefins, and volatiles. The biogas is separated from water and volatiles, produced by deoxygenation processes, in a three phase pressure vessel. The more valuable products of benzene, toluene, and xylenes are then separated from the high-boiling components.

The proposed design converts 400,000 metric tons of wood to 17.4 million kilograms of a BTX mixture per year, including 4.6, 7, and 3.3 million kilograms per year of benzene, toluene, and xylenes, respectively. In addition, 345 GWh of electricity is produced yearly as a byproduct.

The required total permanent investment for this project is $93 MM. At a discount rate of 10% and BTX sale price of $1.1/kg, the base case net present value (NPV) is $(157 MM) and the expected ROI is -20%. The result of this base case analysis suggests that this project should not be further pursued. The best case scenario assumed double the yield of BTX at a sale price of $1.54/kg and a renewable fuel credit of $1.01/gal, resulting in a NPV of $506 MM, an IRR of 70%, and a ROI of 81%. The economic feasibility of this project is also sensitive to the availability and price of biomass, as well as the catalyst degeneration rate within the system.
2. INTRODUCTION
2.1 Project Motivation

Fluid catalytic cracking (FCC) is a process used in oil refineries to convert high boiling hydrocarbon fractions of crude oil to more valuable fractions of gasoline and olefinic compounds. As depicted in Figure 2.1, the FCC process vaporizes and breaks long-chain molecules of high-boiling hydrocarbon liquids into smaller molecules by contacting the feedstock with a fluidized, powdered catalyst at a high temperature and moderate pressure. The products of the FCC process are used by all major oil and gas companies to serve the world’s growing energy demands and as petrochemical feedstocks, respectively.

![Figure 2.1: Schematic of FCC process [1].](image)

The concept behind the FCC process has recently been applied to converting a different type of feedstock, biomass, into valuable syngas. The biomass feed type ranges from wood to corn stover, as well as switchgrass and sugarcane bagasse. The advantage of using biomass is that any type of biomass can be used as a feedstock, and the cracked products are similar to those
produced by the FCC process. The adapted process, referred to as biomass fluidized catalytic cracking (BFCC), is a renewable one that is carbon neutral over the lifetime of the biomass.

The BFCC process applies similar concepts as FCC. In BFCC, biomass of particle size on the micron scale is contacted with a hot catalyst at moderate pressures. Carrier gas, often nitrogen or a recycle stream of volatile products, fluidizes the solid particles. A catalyst then breaks down the components of the biomass into aromatic and olefin vapor products. Olefins and aromatics are the building blocks for a wide range of materials. Olefins are used in plastics, resins, fibers, elastomers, lubricants, synthetic rubber, gels and other industrial chemicals. Aromatics are used for making dyes, polyurethanes, plastics and synthetic fibers [2].

The reaction kinetics of the BFCC process are often much more complex than those of FCC because the composition of the products are sensitive to the reaction conditions and the lignocellulosic composition of the feedstock. In BFCC, biomass undergoes fast pyrolysis in the presence of a catalyst. Pyrolysis occurs at high temperatures and moderate pressures with a residence time of only a few seconds; it also requires high heating and high heat transfer rates with a finely ground biomass feed [3]. These conditions allow the catalyst to interact with the biomass in such a way as to selectively form aromatic and olefin products. The product distribution is also affected by the composition of the biomass, which differs between wood and corn stover, for example. Biomass is composed of cellulose, a linear polymer of glucose, hemicellulose, an amorphous chain of glucose, and lignin, a complex structure of aromatic and alcoholic compounds. Cellulose accounts for around 40-60% of lignocellulose, while hemicellulose and lignin each account for 20-35% [4]. The BFCC process often utilizes an aluminosilicate zeolite catalyst to “crack” the biomass components into smaller aromatic and olefin compounds, as depicted in Figure 2.2.
Zeolites are microporous solids with a very regular pore structure, as shown in Figure 2.3, that have the ability to selectively sort molecules based on size exclusion. The maximum size of a molecule that can enter the pores of a zeolite is controlled by the dimensions of the channels. The zeolite catalyst has been found to be the most effective at decreasing the formation of oxygenated compounds in the BFCC process [4].
The porous structure of a zeolite can accommodate a number of different cations, including Na\(^+\), K\(^+\), Ca\(^{2+}\), Mg\(^{2+}\) and others. These positive ions are rather loosely held and can readily be exchanged with a hydrogen bonded to a carbon atom, creating carbocation intermediates. These intermediates reorganize to form aromatic products. The zeolite’s mechanism of action stems from its catalytic acid sites. Although the exact reaction mechanism of catalytic pyrolysis is still unknown, the process is thought to proceed first through thermal de-polymerization and then deoxygenation. Catalytic pyrolysis of biomass produces large amounts of carbonaceous material in the form of thermal and catalytic coke. Catalytic coke, or char, is generated from both direct thermal decomposition of biomass and secondary reactions of pyrolyzed biomass vapors. Coke is formed during the catalytic reaction of biomass-derived oxygenates. While char is mainly deposited on the external surface of the catalyst, coke infiltrates the inner pore structure of the catalyst. Char and coke decrease the conversion efficiency of catalytic pyrolysis and deactivate the catalyst by depleting its acid sites [4]. The profitability of the proposed BFCC process is therefore sensitive to the lifetime of the catalyst.
The economic feasibility of the BFCC process is also dependent on an abundant availability of biomass input. Biomass is readily available in the U.S., and in such excess that it is characterized as a non-food energy source. According to ORNL, biomass accounted for 4.1% of total primary energy consumption in 2009, compared to that of coal, natural gas, and petroleum with 21%, 25%, and 37%, respectively [6]. However, there has been a substantial rise in biomass and biofuel usage over the last several years. According to BP’s Statistical Review, energy production from biomass and biofuels have more than doubled from 2002 to 2012, rising from 16 millions of tons oil equivalent (Mtoe) to 41 Mtoe [7]. This pattern of increased biomass usage is expected to continue, with ORNL predicting biomass feedstock consumption to increase 76% from 129 to 226 MM dry ton/yr by 2030, as shown in Table 2.1 [6].

<table>
<thead>
<tr>
<th>Source</th>
<th>Current</th>
<th>2017</th>
<th>2022</th>
<th>2030</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forest</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuelwood</td>
<td>38</td>
<td>72</td>
<td>98</td>
<td>108</td>
</tr>
<tr>
<td>Mill residue</td>
<td>32</td>
<td>58</td>
<td>39</td>
<td>42</td>
</tr>
<tr>
<td>Pulsing liquors</td>
<td>45</td>
<td>52</td>
<td>54</td>
<td>58</td>
</tr>
<tr>
<td>MSW sources</td>
<td>14</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Total forest</td>
<td>129</td>
<td>182</td>
<td>299</td>
<td>226</td>
</tr>
<tr>
<td>Agriculture</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethanol</td>
<td>78 (108)</td>
<td>88 (127)</td>
<td>88 (127)</td>
<td>88 (127)</td>
</tr>
<tr>
<td>Biodiesel</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>MSW sources</td>
<td>7</td>
<td>11</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Total agricultural resources currently used</td>
<td>85 (118)</td>
<td>103 (142)</td>
<td>103 (142)</td>
<td>103 (142)</td>
</tr>
<tr>
<td>Total currently used resources</td>
<td>214 (247)</td>
<td>285 (342)</td>
<td>312 (351)</td>
<td>329 (368)</td>
</tr>
</tbody>
</table>

The potential for converting biomass feedstock in this BFCC process is substantial, but is still limited by low conversions to valuable products and high catalyst-to-biomass requirements. This design uses a biomass feedstock of wood chips due to the large capacity available in the southeastern portion of the U.S, as discussed in the “Other Considerations” section. The goal of
this project is to convert non-food source energy resources that are available in excess into more valuable aromatic products. The full scope of this project is outlined in the project charter.
2.2 Project Charter

**Project Name:** Fluidized Catalytic Cracking to Convert Biomass to Fuels

**Project Champions:** Dr. Matthew Targett, Dr. Talid Sinno, Prof. Leonard Fabiano

**Project Leaders:** Stephen Boust, Mo Green, Serena Machi

**Specific Goals:** Design a process to increase the utilization of domestic biomass residues as feedstock for producing bio-derived BTX and electric power via catalytic fast pyrolysis. The desired plant capacity is 400,000 dry tons/yr.

**Project Scope:**

*In-scope:*
- Determine suitable biomass feed and feasible input capacity
- Impact of renewable fuel credits
- Base and best case profitability analysis
- Economic sensitivity to catalyst lifetime

*Out-of-scope:*
- Predictive modeling of biomass product distribution based on lignocellulosic makeup
- Manufacture of catalyst
- Specific handling of waste streams
- Detailed process control design

**Deliverables:**
- Process Design with Energy & Mass Balances
- Technical Feasibility Assessment
- Economic assessment

**Timeline:**

*Milestones*
- February 3: Preliminary material balance and computer-drawn block flow diagram
- February 24: Base case material balance and computer-drawn process flow diagram
- March 17: Detailed equipment design for a key process unit
- March 24: Major equipment designed
- March 31: Finances completed
- April 7: First draft of written report
- April 14: Final draft of written report
- April 21: Oral design report presentation
2.3 Innovation Map

The innovation map shown in Figure 2.4 outlines the value chain of this process. The proposed design converts biomass to valuable aromatic compounds, which can help reduce the chemical industry’s dependence on fossil fuel-derived BTX. The biomass is non-food source available in excess in the U.S., making this a renewable process. In addition, this process is somewhat carbon-positive, taking into account harvesting and transportation of the biomass, but in terms of running the plant, no new carbon is produced during the lifetime of the biomass. This is because greenhouse gases were consumed during the biomass’ growth period. This process has been optimized to make use of the systems internal heat network, which results in the production of a large amount of steam. This steam is used as an energy source for the plant and also to fulfill the plant’s electricity requirements.

![Innovation Map](image-url)

**Figure 2.4:** Innovation map of fluid catalytic cracking process to convert biomass to BTX.
3. CONCEPT STAGE
3.1 Market Analysis

The group of petrochemicals benzene, toluene, and xylene, often referred to as BTX, has traditionally been produced as a byproduct from the catalytic cracking of naphtha in petroleum refineries. BTX can also be derived from the steam cracking of hydrocarbons and as a byproduct of coal refining and ethylene production. Because BTX is currently produced predominantly as a byproduct from other processes, its production capacity depends directly on the demand for its precursors. Using biomass as a feedstock would reduce the chemical industry’s dependence on fossil fuels and create an independent commodity for bio-derived BTX.

The value of BTX stems from the wide use of its derivatives, which are used in the construction, automotive, apparel, appliance, computer, electronics, and packing industries [8]. BTX comprise three of the seven primary chemical feedstocks used by the chemical industry to make an array of products such as automobile tires, nylon, laundry detergent, polyester clothing and packaging. In addition, equally significant volumes of toluene and xylenes are blended into gasoline to boost octane ratings [2]. Half of the benzene produced globally in 2010 was used as a precursor for styrene, which is further polymerized to produce products including rubber, plastic, insulation, fiberglass, pipes, automobile and boat parts, food containers, and carpet backing [9]. The wide range of end uses for BTX is outlined in Figure 3.1.
The market for BTX is a global one, with demand especially anticipated to grow in Asia and the Middle East. China emerged as the leading consumer of petrochemicals in 2013 and accounted for over 25% of the global demand in that year. In addition to being the largest market, China is anticipated to be the fastest growing market for petrochemicals, expanding at a high compound annual growth rate (CAGR) between 2014 and 2020. Initiatives taken by the government of China to boost the petrochemicals market coupled with growth in end-use industries in the region is expected to significantly drive the market during the forecast period [11]. The rest of Asia Pacific was the second-largest consumer of petrochemicals in 2013. Market growth in this region, especially in India, is driven by an increase in demand for downstream products. Demand for petrochemicals in the Middle East and Africa is primarily led
by rapid capacity additions in the region. The market for petrochemicals in North America and Europe is estimated to grow at moderate rate during the forecast period.

Benzene, toluene and xylenes (BTX) are a $120-billion global market, historically growing at rates greater than the global GDP. IHS Chemical reports that global demand for benzene increased to 43.7 MM metric tons in 2013, and is expected to increase by around 3% in the next five years [8]. Transparency Market Research estimated that the global petrochemicals market was valued at $558.61 billion in 2013 and predicts that it will reach $885.07 billion by 2020, expanding at a CAGR of 6.8% from 2014 to 2020 [11]. As shown in Figure 3.2, Roland Berger Strategy Consultants predicts that the growth of the petrochemicals market will reach around 1.3 trillion by 2030 [12].

![Diagram showing demand for petrochemicals by region, 2000, 2010, and 2030](image)

**Figure 3.2:** Demand for petrochemical by region, 2000, 2010, and 2030 [12].

This new BFCC process has the potential to reduce or eliminate the chemical industry's current reliance on fossil fuels to make industrial chemicals worth an estimated $400 billion annually [2]. BTX is purchased by well-known oil and gas companies such as BP, Chevron Phillips, Dow, DuPont, ExxonMobil, Shell, and Sunoco for use as a fuel additive or as a petrochemical feedstock [13]. The proposed design produces approximately 4,600 tons
benzene/yr, which accounts for about .01 % of the global benzene production in 2013. With advances in fluidized catalytic cracking technology and catalyst effectiveness, the efficiency of the proposed BFCC process has potential to significantly account for global BTX production.

3.2 Competitive Analysis

According to estimates by the U.S. EIA, biomass power generation in 2012 was about 58,000 GWh, equivalent to about 4% of US coal fired power generation, which consumed between 50-100 million tons of biomass depending on the type and energy content of the biomass being used [14]. Another study by ORNL reports that an additional 250 million tons of dry biomass is potentially available at $60 per dry ton or less [6]. Assuming that this new BFCC technology could be deployed in such a way to utilize an additional 250 million tons of biomass, it could produce 156 million bbls per year of renewable BTX products. This additional output could replace approximately 22% of the global BTX consumption in 2013.

As discussed earlier, BTX has traditionally been produced as a byproduct of naphtha catalytic cracking, steam cracking of hydrocarbons, coal refining, and ethylene production. As shown in Figure 3.3, the value of products produced by gas-to-liquid (GTL), coal-to-liquid (CTL) and biomass to liquid processes was worth $8.4 billion in 2014 [2].
This total is expected to grow from $8.6 billion in 2015 to $11.8 billion in 2020, with a CAGR of 6.5% from 2015 to 2020 [8]. The value of products produced by GTL processes is expected to grow from $5.6 billion in 2015 to $7.7 billion by 2020, with a CAGR of 6.6%. The total CTL business is expected to account for $3 billion worth of product in 2015 and $4 billion in 2020, increasing at a CAGR of 5.9%.

There are already a few companies implementing catalytic fast pyrolysis technology to convert biomass to petrochemicals, most prominently Anellotech, Envergent, and KiOR. Anellotech’s process is compatible with various renewable feedstocks, including palm wastes, bagasse, corn stover, and wood. Using its proprietary catalyst, Anellotech’s CFP process enables biomass to be converted in a fluidized-bed reactor into commercially viable aromatics, principally benzene, toluene and xylenes (BTX). Anellotech's products are less expensive to manufacture than their identical petroleum-derived counterparts, which is achieved by performing all chemical conversions in one reactor and an inexpensive catalyst [2].
Envergent is a joint creation between UOP, a Honeywell company based out of the United States, and Ensyn, a Canadian based company that has developed and patented a Rapid Thermal Processing (RTP) technology. RTP is a fast thermal process in which biomass, usually forest residuals or agricultural by-products, is rapidly heated to approximately 500°C in the absence of oxygen. A tornado of hot sand vaporizes the biomass, which is then rapidly quenched, typically yielding 65-75 wt% RTP green fuel. This pourable liquid can then be used as fuel for industrial heat or electrical generation, or it eventually can be further upgraded to produce transportation fuels. Envergent’s RTP technique, although effective at converting biomass to green fuels, is done in the absence of catalyst which is dissimilar to our process which utilizes a zeolite catalyst [15].

KiOR’s process utilizes its proprietary catalyst systems with a biomass feed in an FCC-type system to generate gasoline and diesel blendstocks. The company’s approach is more efficient over traditional biofuels producers because using their biomass fluid catalytic cracking method combined with the proven nature of catalytic cracking technologies has lower capital and operating costs, creating significant cost advantages. The company converts sustainable, low cost, non-food biomass into hydrocarbon-based renewable crude oil which is passed through a hydrotreater to be refined into these blendstocks. All parts of the products are used in some way; the light gases generated are burned to create steam and generate electricity while the crude is condensed and refined [16]. KiOR was able to operate this process on an industrial scale successfully for some time, but just recently went bankrupt in the November of 2014.

The competitive landscape within this renewable petrochemical industry can be analyzed using a tool called Porter’s Five Forces. This tool analyzes the level of competition within an
industry by gauging the threat of new entrants, substitutes, and established rivals as well as the bargaining power of suppliers and buyers [17].

The threat of new entrants is affected by high barriers to entry, which in the renewable petrochemical industry may come in the form of patents and government policies. If government policies such as renewable credits are in place, the threat of new entrants may be high as many new, potentially profitable projects may be pursued. Any successful company in this industry has various patents protecting their processes, which would make the threat of new entrants low.

The threat of substitute products will be high for this project, as FCC is already an established process that results in high conversions to valuable products. Other factors affecting threat of substitutes includes perceived level of product differentiation and buyer switching costs. In theory, the switching costs to BTX generated from BFCC would be negligible as oil and chemical companies could purchase the product at a competitive price. As long as the BFCC derived BTX proves to be just as chemically valuable as the one from FCC, the perception level of the product should not increase the threat of substitute products.

The threat of established rivals will likely be low, as there are few companies operating BFCC processes on an industrial scale. Anellotech is currently operating a pilot plant, but as it has yet to achieve profits on an industrial scale, rivals should not prove a viable threat.

The bargaining power of suppliers will likely be low in this industry, as non-food source biomass such as wood is available in excess throughout the country. However, buyers may have a high bargaining power as the same product can be bought from FCC companies.

Overall, the industry outlook for this BFCC process looks promising, despite the recent decline in the market value of BTX.
3.3 Preliminary Process Synthesis

This design was adapted from the results of a study conducted by Carlson et al. from the University of Massachusetts Amherst titled “Production of Green Aromatics and Olefins by Catalytic Fast Pyrolysis of Wood Sawdust” [18]. The study analyzed the composition of wood sawdust in terms of its lignocellulose breakdown on a weight percent basis of cellulose, hemicellulose, and lignin as well as on an atomic basis. The study reported the yields of the catalytic fast pyrolysis experiment on a carbon basis, as summarized in Table 3.1.

Table 3.1: Summary of product yields reported by Carlson et al [18].

<table>
<thead>
<tr>
<th>Component</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Overall</strong></td>
<td></td>
</tr>
<tr>
<td>Aromatics</td>
<td>11.0</td>
</tr>
<tr>
<td>Olefins</td>
<td>8.2</td>
</tr>
<tr>
<td>Methane</td>
<td>4.5</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>26.3</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>8.1</td>
</tr>
<tr>
<td>Coke</td>
<td>30.2</td>
</tr>
<tr>
<td><strong>Aromatics</strong></td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>23.1</td>
</tr>
<tr>
<td>Toluene</td>
<td>30</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>1.2</td>
</tr>
<tr>
<td>m-Xylene &amp; p-Xylene</td>
<td>12.0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>1.9</td>
</tr>
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</tr>
<tr>
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<td>4.0</td>
</tr>
<tr>
<td>Indene</td>
<td>7.1</td>
</tr>
<tr>
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</tr>
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</tr>
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<td>1.9</td>
</tr>
<tr>
<td>Butadiene</td>
<td>5.0</td>
</tr>
</tbody>
</table>
The kinetics of this process are complex and often difficult to model and therefore were not presented in the study. Due to the lack of accurate reaction kinetics, the RYIELD process unit was chosen to model the process on an industrial scale. For a different biomass feedstock, such as corn stover, with a known lignocellulosic composition and product distribution, this process design can be retrofitted to model its industrial-scale manufacture. Moreover, if the reaction kinetics of a catalytic fast pyrolysis process can be accurately modeled, the RYIELD can be replaced with a RSTOIC unit to yield a product distribution from known input components.

3.3.1 Reactor Yield and Mass Balance

The selectivity’s for products coming out of the BFCC riser were adapted from Carlson’s study of pinewood undergoing CFP [18]. The paper reported the yield of the carbon pyrolysis products on a carbon yield basis. These carbon yields were used to determine the mass of each carbon-bearing product leaving the BFCC riser. The calculated mass flow leaving the riser did not add up to the mass of the biomass feed. Because the yields were on a carbon basis, water was not included, yet this is an important byproduct of the pyrolysis process. The missing mass was therefore assumed to be water. The mass yield for each compound could then be calculated for use in the RYIELD block in the Aspen Plus simulation. The carbon yield and the mass yield used as the basis for these calculations are shown in Table 3.2.
Table 3.2: Carbon and Mass Yields used in this BFCC design.

<table>
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<tr>
<th>Products</th>
<th>Carbon Yield</th>
<th>Mass Yield</th>
</tr>
</thead>
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<tr>
<td>Benzene</td>
<td>2.54</td>
<td>0.014</td>
</tr>
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<td>Toluene</td>
<td>3.30</td>
<td>0.018</td>
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<td>0.0007</td>
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<td>m-Xylene</td>
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<tr>
<td>p-xylene</td>
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<td>0.0036</td>
</tr>
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<td>Carbon Monoxide</td>
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<tr>
<td>Water</td>
<td>-</td>
<td>0.28</td>
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</tbody>
</table>

3.3.2 Catalyst Lifetime

The lifetime of the catalyst used in the FCC and BFCC process is an important factor in ensuring the desired product formation and in maintaining the economic feasibility of the process. During operation, the coke and char get deposited on the acid sites of the catalyst, thereby deactivating it over time. However, combustion of the coke deposited on the ZSM-5 catalyst can lead to almost perfect regeneration of the catalyst.

In typical FCC processes, the catalyst makeup rate is approximately 0.25 lb. catalyst/barrel of feed. This leads to purge fractions of less than 0.01%. However, the biomass fluidized catalytic cracking process designed in this report differs from a typical FCC process in
a few key distinctions. The first is the amount of coke that is produced as a percentage of input. When biomass is used as a feed, approximately 30% of the carbon, or 15% percent by mass, of the feed is deposited onto the catalyst as coke. Typical FCC processes result in a coke yield of 3-8% by weight. To account for the increase in coke production in the process designed in this report, the purge fraction of catalyst was increased to 0.002, which results in 215 kg/hr of catalyst being purged from the process. This is very expensive, and further testing should be done to determine the rate of catalyst degradation during a BFCC process.

3.3.3 Catalyst Regeneration with Acid Wash

The proposed design implements a combustor to regenerate the ZSM-5 catalyst, as is done in the traditional FCC process. Anellotech, Inc. has patented a process for the regeneration of the catalyst used in a fast pyrolysis process, as shown in Figure 3.4. The patent details a process in which the catalyst is regenerated by first passing through an oxidative regenerator, followed by an additional step in which it is contacted with a dilute acid or base solution before being separated from the waste solution and returned to the reactor. The acid wash replaces the depleted Brønsted acid sites, which are integral to the zeolite’s ability to crack the biomass into aromatic compounds.
The patent suggests using ammonium salts such as ammonium nitrate, ammonium acetate, ammonium oxalate, or ammonium phosphate as the washing solution. Once the catalyst has been washed, it may have ~79% of the acid sites as it would have before undergoing catalytic fast pyrolysis.

The Anellotech patent also found that catalyst can be successfully used for CFP with a significant percentage of contaminants; for this reason and to avoid procuring additional capital costs, it was decided that the catalyst be regenerated in the traditional way with only an oxidative regenerator. If the acid wash were to be added to the process design, extra equipment in the form of a holding tank for the solution, a vessel with mixing capacities, and a solid/liquid centrifuge.
3.3.4 Use of Spray Condensers to Extract Liquid Product

Spray condensers were explored to extract liquids out of the pyrolysis gas stream, S304, instead of using a traditional compressor. Compressing the pyrolysis gas is very costly due to the high flow of gas, leading to a large power requirement. Replacing the compressor with a spray condenser could reduce this cost achieved the same desired output.

The spray condenser unit using nozzles to spray a coolant into a vessel whose inlet is a vapor stream. As shown in Figure 3.5, the cooling water is sprayed into the top of the column, at which point it is contacted with the hot vapor stream. The water and vapor stream can be fed either concurrently or countercurrently, but the condensed liquid stream exits out the bottom of the unit and is pumped to its next destination.

![Figure 3.5: Schematic of spray condenser unit [20].](image)

While this method would more readily condense and cool the vapor stream, it would also introduce a large amount of water into the system, which would need to be decanted and then treated for the trace amount of aromatics that would condense into the liquid phase. This process would require a spray condenser, spray tower, flash cooler, and at least two pumps, adding to the
already large capital costs of this project [21]. The use of cooling water would also accrue an additional capital cost.

3.3.5 Extractive Distillation for Purification of BTX Product

Extractive distillation was explored to further purify the BTX mixture coming out of the distillation column. The BTX mixture contains 6% styrene, 2% ethylbenzene, and 1% phenol. The BTX mixture would have to be sold at a discount unless these impurities are removed, so extractive distillation was investigated. Extractive distillation is characterized by the distillation of a mixture with low relative volatility in the presence of a miscible, non-volatile, high-boiling solvent. Mixtures with a low relative volatility cannot be separated with simple distillation because the components will evaporate at close temperatures, thereby hindering a normal distribution of products. The solvent works to enhance the volatility difference between the components, letting less volatile components flow to the bottom of the distillation column and the more volatile component come out the top. The extractive component is recovered in the bottoms stream [22]. The process yields aromatic purities of 99.99 wt% and yields of more than 99.9 % [23].

Although extractive distillation is often used in practice to attain a pure BTX product, this design focuses on the conversion of biomass to valuable aromatic compounds, and therefore less on the purification of the product stream. Additional capital costs would also be incurred for the procurement of the solvent, and as this process is already capital intensive, extractive distillation was not chosen as the method of product purification.

3.3.6 Co-sale of Propylene

Additional revenue may also be captured by the co-sale of refinery grade propylene, which is produced in the CFP reaction in the BFCC riser. Refinery grade contains approximately
70 wt% propylene with other aromatics mixed in and was selling at a price of $.77/kg in July of 2009 [24]. A majority of the propylene in the system is contained within the volatile stream that comes off the top of the three phase flash drum. The volatile stream contains non-condensable gases including propylene, carbon dioxide, and carbon monoxide. Assuming 95% of the propylene can be extracted with a similar polymer grade breakdown from the three phase flash drum, 556 kg/yr would be recovered, generating an additional annual revenue of $7,220,000. However, this revenue would be offset by the additional capital costs required to purchase the equipment and cover operating costs.

### 3.3.7 Process Design Influences

The proposed process design is the composite of various other process designs as proposed in patents and technical papers. The initial influence for this BFCC process comes from the industrial process design of KiOR, which is detailed in the company’s patent, titled “Two-Stage Reactor and Process for Conversion of Solid Biomass Material” [25]. As shown in Figure 3.7, KiOR’s process begins by using lift gas (16) to fluidize biomass particles (14), which contact catalyst particles (20) in a two-stage reactor (1). The solid and vapor products exit out of the top of the second stage of the riser and are fed to the cyclone (26). The coke and catalyst exits the bottom of the cyclone into a regenerator (44). The valuable liquid bio-oil is then recovered in the bottoms stream (34) of a distillation column (32).
While KiOR’s process served as the basis for this design, other sources were also used in developing the proposed design. Shell Oil Company developed a BFCC process, as detailed in the patent entitled “Process for Converting a Solid Biomass Material” [26]. This patent offered insight into the particle size distribution of the biomass that would affect the greatest conversion to valuable products. In addition, this patent offered suggestions for the different types of carrier gas that could be used. Another patent that offered valuable ideas is one from Anellotech, Inc. entitled “Fast Catalytic Pyrolysis with Recycle of Side Products” [27]. This patent offered greater detail into the solid handling required for the process as well as a scheme for using non condensable vapor products in a recycle stream as the carrier gas for biomass in the reactor.
The previously discussed patents offered valuable conceptual ideas, but more process oriented sources were also used to try and translate these ideas in Aspen to more accurately model the process on an industrial scale. For example, a study conducted by Yan et al. offered ideas for integrating a heat network in the process [28]. Finally, a process designed by Iowa State University included a waste heat boiler, which was also integrated into this process design [29].

3.4 Assembly of Database

This design project was modeled using Aspen Plus V8.6. To avoid errors associated with compatibility, all simulations of this project should be run with V8.6 of Aspen Plus.

This equilibrium simulation used the Soave-Redlich-Kwong (SRK) equation of state to model vapor and liquid thermodynamics. The SRK equation of state does not accurately model system thermodynamics near the critical points of the components, which is often the circumstance in petroleum refining. This means that the SRK does well to model mixture parameters of hydrocarbons during condensation process, which occurs in the proposed design. It is also important to note that the “STEAMNBS” was specified as the steam type, which is an equation of state for water. Also, the sub-stream type was changed to “SOLID” for the compounds modeling wood, catalyst, and coke.

As biomass is a solid made up of complex lignocellulosic networks, various model compounds were chosen to represent the lignocellulosic makeup of the biomass feedstock. Biomass is generally composed of lignocellulose, cellulose, and hemicellulose. Both cellulose and hemicellulose are polymers of glucose, the former linked in a linear chain and the latter in an amorphous structure. Both cellulose and hemicellulose were modeled with the compound cellobiose, a disaccharide consisting of two linked glucose molecules. Lignin is a complex
polymer of aromatic alcohol, allowing it to serve as the structural support for cell walls. Two compounds, diphenyl ether and guaiacol, were used to model lignin in this simulation. Diphenyl ether consists of two phenyl rings bonded in an ether orientation, thereby making it a good representation of lignin’s aromatic qualities. With an alcohol group extended off an aromatic ring, guaiacol serves as a good representation of lignin’s alcoholic makeup [2].

While these model compounds well represent the chemical makeup of wood, their thermodynamic properties differ slightly from those of real wood. The overall process can be viewed essentially as a combustion reaction, with biomass as the input and volatile compounds carbon dioxide and carbon monoxides as the output. In analyzing the thermodynamics of this overall combustion process, the heating value of the model compounds is less than that of real wood, whose lower heating value is approximately 19,000 kJ/kg. This disparity enlightens the fact that this process would likely generate more heat and therefore more electricity when operating with real wood as the input.

There were a few key unit operations that required multiple units to be modeled in Aspen, although in practice would be operated in a single process unit. For example, the biomass was prepared for pyrolysis by first being dried and then crushed. Many conventional process now use a process equipment called “PulverDryers” to simultaneously dry and grind the biomass. In addition, the RYIELD block could not be modeled in a way so as to have all inputs feed directly to the reactor. Because the product yield is specified, any recycle loop containing compounds in the product stream cause an error in the simulation convergence. The recycle loops of the volatile products, which are used as co-carrier gases, as well as the catalyst recycle, were mixed after the reactor before being fed into the solid/vapor cyclone.
4. PROCESS FLOW DIAGRAMS AND MATERIAL BALANCES
4.1 Overall Process Flow Diagram

Figure 4.1: Overall process flow diagram for the proposed process to convert biomass to fuels.
4.2 Block 100: Biomass Preparation

Figure 4.2: Process Flow Diagram for the solids handling section.
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<th>S104</th>
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Figure 4.3: Process Flow Diagram for the pyrolysis & catalyst regeneration section.
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4.4 Block 300: Product

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4.5 Block 400: Heat Integration

Figure 4.5: Process Flow Diagram for the heat integration section.
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Mass Frac

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4.6 Block 500: Electricity Generation

Figure 4.6: Process Flow Diagram for the electricity generation
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5. PROCESS DESCRIPTIONS
5.1 Process Overview

![Block Flow Diagram for Fluidized Catalytic Cracking to Convert Biomass to Fuels process](image)

**Figure 5.1:** Block Flow Diagram for Fluidized Catalytic Cracking to Convert Biomass to Fuels process

Figure 5.1 shows the overall process design, with each process section boxed and labeled. Important mass and energy flows are shown connecting the different process sections. Solid lines represent mass transfer and dashed lines represent energy transfer. The process begins with the biomass preparation. The plant will receive bulk biomass in the form of wood-chip waste from wood processing facilities. This biomass is estimated to have a 30% moisture content. Process section 100 reduces the particle size of the biomass as well as reducing its moisture content to 5%. The energy required for drying is obtained via hot air heated in process section 400, the heat exchange network. The treated biomass is then able to enter the catalytic fast pyrolysis unit, CFP and then have the solid and vapor products be separated in the catalyst regeneration step. These two processes make up process section 200. The vapor products are then sent to the product separation block, process section 300, where the valuable aromatic compounds are separated from the less valuable carbon bearing products. These less valuable products are sent to process
section 400 so that their chemical energy can be turned into heat to produce steam in process section 500.

5.2 Process Section 100: Biomass Preparation

Process section 100 is the section where the solid, raw biomass is processed so that it can be brought down to a particle size acceptable for fluidization and be dried. A schematic of this process section can be seen in Figure 4.2 on page 40. 1,500 tons of biomass with a moisture content of 30% are stored in hoppers before entry into the solids handling system. This represents one day’s worth of biomass processing. The biomass is split into two streams so that it can be dried and pulverized. A third processing stream is available as a backup.

Each processing stream contains 31,000 kg/hr of wet biomass. The biomass enters a dryer where it is exposed to 300 °C air so that the wood can be brought up to 175 °C and brought down to a moisture content of 5% by weight. Screw feeds are used to transport the 23,000 kg/hr of dry biomass into a hammer mill. The hammer mills pulverize the biomass so that it exits at a particle size between 100 and 500 microns in diameter. The pulverized wood streams are combined and sent via a screw feeder into process section 200 via stream S115 so that it may enter the BFCC riser.

5.3 Process Section 200: Pyrolysis & Catalyst Regeneration

Process section 200 is the section in which the main chemical operations occur. A schematic of this process section can be seen in Figure 4.3 on page 42. It begins with dried, pulverized biomass entering the bottom of the fluidized catalytic cracking unit, R-201, to be
introduced to the alumina-silicate catalyst entering the fluidized bed in stream S214. Both the solid catalyst and biomass feed are fluidized using recycled volatile products from the BFCC reaction via stream S216 at 600 °C. The fluidization medium consists primarily of non-reactable gases: 80% by mass carbon monoxide and carbon dioxide. The remaining 20% consists of methane, propylene and butane. It is likely that that these compounds would undergo aromatization by the ZSM-5 catalyst. However, the conversion to valuable products from this feed is currently unknown and thus the small chain hydrocarbons are assumed to be unreactive. The biomass is exposed to the catalyst for an average of 2.5 seconds within the reactor before exiting the top of the riser with the fluidized catalyst and BFCC products.

Within the riser, the elevated temperature of the reactor facilitates the pyrolysis of the biomass particles. The cracked particles are then synthesized into aromatic compounds inside of the pores of the ZSM-5 catalyst. The coke is assumed to gather on the catalyst particles and thus be fluidized by the carrier gas and carried out of the reactor with the catalyst and BFCC products.

The product stream coming out of the reactor is blown into a cyclone separator by the blower, B-201. The cyclone separator block, Cy-201, separates the gaseous and solid components using the difference in densities. The stream enters the cylindrical cyclone vessel tangentially and the solid particles fall to a conical collection section of the cyclone while the volatile components remain at the top. The volatile products leave the cyclone via stream S203 to head into process section 300 for product separation. The solid stream coming out of the cyclone is estimated to have 7,640 kg/hr of coke compared to 100,000 kg/hr of catalyst and heads to the catalyst regeneration units.

A small fraction, 0.2%, of the catalyst coming of the cyclone is assumed to lose its functionality with each pass through the reactor, so a purge is taken off via stream S205. This
The purge is also assumed to remove any unreactive biomass char or impurities that are present in the reactor. The remainder of the coke and catalyst stream enters a combustion reactor, R-202, to remove the coke from the catalyst.

Inside of the combustion reactor, the carbon coke is exposed to excess oxygen in the form of air to completely regenerate the catalyst by oxygenating coke to CO\textsubscript{2}. Excess air is used so that the nitrogen present and excess oxygen can act as a diluent to absorb much of the heat that is released from the highly exothermic combustion of coke. This is done so that the catalyst does not reach a temperature above the level where the catalyst may start to deactivate. The amount of air used is 390 kg/hr, representing a stoichiometric excess of 4.5 times the amount of oxygen needed.

The regenerated catalyst and flue gases coming out of the combustion reactor are fed into a second cyclone separator so that the catalyst can be separated from the flue gases. The hot gases leave the top of the cyclone and are fed into a heat exchanger network in process section 400 via stream S212 to generate steam. A second stream consisting of regenerated catalyst leaves the bottom of the cyclone. The regenerated catalyst is combined with 215 kg/hr of fresh catalyst in stream S213 to replace the small fraction that deactivated. The recycled catalyst is then fed into the BFCC riser. The hot catalyst has enough energy to heat the biomass to 600 °C.

5.4 Process Section 300: Product separation

Process section 300 is the process section where the valuable aromatic components are separated from the less-valuable multi-ring aromatics and non-condensable volatile components such as CO\textsubscript{2}, CO and olefins. A schematic of this process section can be seen in Figure 4.4 on page 45. The separation train begins with a pressurized flash drum at low temperatures that
separates the product mixture into volatile components, organic aromatics and water with trace amounts of aromatics. The organic stream then enters a distillation column to extract the higher value BTX compounds from the lower value multi-ring aromatics. A second distillation column is then used to separate the phenol from the high-boiling, valuable aromatics. As each stream is removed, it is sent to a combustion reactor in process section 400 so that the heating value of the stream may be realized.

Process section 300 is connected to process section 200 by stream S301, which carries the gaseous components coming from the first cyclone. The gases enter this section at 600 °C and need to be cooled and pressurized before entering the flash drum. The gases are first brought down to 80 °C by heat exchanger HX-301. The BFCC products enter the tube side of the heat exchanger and purified water is used in the shell side to generate 13,000 kg/hr of high pressure steam at 411 °C.

The cooled products are then pressurized and condensed in units C-301 and Cn-301 respectively. C-301 pressurizes the BFCC product stream to 9 bar. This also raises the temperature of the gas to 326 °C. The pressurized stream then enters the condenser where its temperature is brought down to 5 °C using chilled water. 15,000 kg/hr of water at 1 °C are used to cool the hot stream to the required temperature.

The cold, pressurized BFCC products then enter the flash vessel, Fl-301, with a flow rate of 52,000 kg/hr to be separated into three streams. Inside the drum, three phases exist: volatile, aqueous, and organic. The volatile products are taken off the top of the vessel via stream S310 carrying 40,000 kg/hr of volatile components and are sent to the BFCC riser to act as a fluidization fluid. The stream consists of 60% by mass CO, 28% CO₂ and the remainder light hydrocarbons such as methane, ethylene, propylene, and butane. At the bottom of the drum, the
liquids will settle and separate into aqueous and organic phases. The organic phase has a lower density than water and so will remain above the aqueous phase. Stream S312 removes the aqueous phase from the bottom of the flash vessel. This stream has a flow rate of 9,230 kg/hr and is composed of 99.9% water with trace amounts of organics and dissolved gases. Stream S313 removes the organic phase from the flash drum to head to a series of two distillation columns for further purification of BTX. The stream has a flow rate of 3,270 kg/hr and the mass fractions of the compounds in this stream can be seen in Table 5.1, with trace amounts of water and dissolved gases.

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<th>Component</th>
<th>Percent Mass Composition</th>
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<td>Toluene</td>
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</tr>
<tr>
<td>Xylenes</td>
<td>14</td>
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<td>Indene</td>
<td>7</td>
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<td>Phenol</td>
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<td>Styrene</td>
<td>5</td>
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<tr>
<td>Carbon Dioxide</td>
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The organic stream leaving the flash vessel then proceeds to enter a distillation column to separate the lighter aromatics from lower-value large aromatic compounds. The distillation column operates based off of the difference between boiling points for the light aromatics and the heavy ones. The boiling points for the compounds present is listed in Table 5.2.

The heavy key for this distillation column is styrene and the light key is ortho-xylene. The column has 27 stages and operates at a lower pressure and higher temperature than the flash drum. An azeotrope exists between water and phenol at high pressure. Because of this, the
styrene, indene and naphthalene leave via the bottoms product, but some of the phenol is carried up the column with the water and leaves with the BTX as an overhead product in stream S316. The high-boiling aromatics leave via stream S317 to the combustor in process section 400.

Table 5.2: Volatilities of components in the organic stream leaving Fl-301

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Stream S316 has a flow rate 2,300 kg/hr and consists of mostly BTX and 4.5% by mass phenol. To eliminate the phenol, the pressure of the stream is reduced so that the azeotrope between phenol and water has a diminished effect and a second distillation column is used. The second column contains only 15 stages and operates at 4.5 bar. The bottoms product of this column has a flow rate of 115 kg/hr and is composed of 70% phenol. The overhead product is the process’ final separation stream and contains 94% BTX and is at 25 °C. Stream S318 takes the overhead product to short term storage before it can be sold.

The reason the flash vessel operates at such high pressures is so that more of the valuable products condense out of the vapor phase. A simple optimization was done to determine the pressure at which the flash vessel would operate. Holding everything else equal, the amount of product coming out of the first distillation column as an overhead product was compared to the
amount of energy consumed to pressurize the BFCC products for varying pressures. To compare revenues versus cost, a price of $1.1 per kilogram and an electricity cost of $0.07 per kWh were used. The increase in bare module cost for the compressor when power consumption increased was not taken into account for this experiment. The results of the optimization experiment are shown in Table 5.3. It can be seen that the operating pressure that yields the highest revenues minus utility cost is 9 bar. However, the optimum operating pressure changes as a function of product price. The same experiment was done with varying product prices and the resulting optimum operating pressure results are shown in the Table 5.4.

<table>
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<th>Flash Drum Operating Pressure (bar)</th>
<th>Product Flow Rate (kg/hr)</th>
<th>Compressor C-301 Power Requirement (kW)</th>
<th>Product Sales ($/yr)</th>
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<td>3</td>
<td>2096.71</td>
<td>2359.223</td>
<td>$ 18,266,507.38</td>
<td>$ 1,307,953.10</td>
<td>$ 16,958,554.28</td>
</tr>
<tr>
<td>4</td>
<td>2167.24</td>
<td>3085.729</td>
<td>$ 18,880,987.30</td>
<td>$ 1,710,728.15</td>
<td>$ 16,170,259.15</td>
</tr>
<tr>
<td>5</td>
<td>2214.48</td>
<td>3681.325</td>
<td>$ 19,292,536.95</td>
<td>$ 2,040,926.59</td>
<td>$ 16,251,610.37</td>
</tr>
<tr>
<td>6</td>
<td>2248.52</td>
<td>4189.575</td>
<td>$ 19,589,129.85</td>
<td>$ 2,322,700.62</td>
<td>$ 16,266,429.23</td>
</tr>
<tr>
<td>7</td>
<td>2274.05</td>
<td>4634.922</td>
<td>$ 19,811,555.57</td>
<td>$ 2,569,600.93</td>
<td>$ 16,241,954.64</td>
</tr>
<tr>
<td>8</td>
<td>2293.67</td>
<td>5032.563</td>
<td>$ 19,982,474.04</td>
<td>$ 2,790,053.09</td>
<td>$ 16,192,420.95</td>
</tr>
<tr>
<td>9</td>
<td>2309</td>
<td>5392.644</td>
<td>$ 20,116,039.10</td>
<td>$ 2,989,681.70</td>
<td>$ 17,126,357.40</td>
</tr>
<tr>
<td>10</td>
<td>2321.14</td>
<td>5722.299</td>
<td>$ 20,221,769.07</td>
<td>$ 3,172,442.56</td>
<td>$ 17,049,326.51</td>
</tr>
<tr>
<td>11</td>
<td>2330.84</td>
<td>6026.752</td>
<td>$ 20,306,312.75</td>
<td>$ 3,341,231.56</td>
<td>$ 16,965,081.19</td>
</tr>
<tr>
<td>12</td>
<td>2338.7</td>
<td>6309.951</td>
<td>$ 20,374,765.29</td>
<td>$ 3,498,237.07</td>
<td>$ 16,876,528.22</td>
</tr>
<tr>
<td>13</td>
<td>2344.98</td>
<td>6574.957</td>
<td>$ 20,429,498.34</td>
<td>$ 3,645,156.18</td>
<td>$ 16,784,342.16</td>
</tr>
<tr>
<td>14</td>
<td>2350.07</td>
<td>6824.194</td>
<td>$ 20,473,838.68</td>
<td>$ 3,783,333.34</td>
<td>$ 16,690,505.33</td>
</tr>
<tr>
<td>15</td>
<td>2354.24</td>
<td>7059.62</td>
<td>$ 20,510,147.85</td>
<td>$ 3,913,853.14</td>
<td>$ 16,596,294.71</td>
</tr>
</tbody>
</table>
Table 5.4: Results of sensitivity analysis for price of product and operating pressure in the flash drum

<table>
<thead>
<tr>
<th>Price of Product ($/kg)</th>
<th>Optimal pressure (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>4</td>
</tr>
<tr>
<td>0.9</td>
<td>5</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
</tr>
<tr>
<td>1.1</td>
<td>9</td>
</tr>
<tr>
<td>1.2</td>
<td>9</td>
</tr>
<tr>
<td>1.3</td>
<td>9</td>
</tr>
<tr>
<td>1.4</td>
<td>10</td>
</tr>
<tr>
<td>1.5</td>
<td>10</td>
</tr>
<tr>
<td>1.6</td>
<td>9</td>
</tr>
<tr>
<td>1.7</td>
<td>9</td>
</tr>
<tr>
<td>1.8</td>
<td>9</td>
</tr>
<tr>
<td>1.9</td>
<td>9</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
</tr>
</tbody>
</table>

5.5 Process Section 400: Heat Integration

Process section 400 is the process section where the energy in all streams not sold as products are taken to generate stream. A schematic of this process section can be seen in Figure 4.5 on page 49. Many of the streams enter this section at elevated temperatures. These streams are used in heat exchangers to provide heat to streams that head into other process units or to generate steam. Many of the side-product streams coming from process sections 200 and 300 contain hydrocarbons that have value as heating components. These streams enter a combustion reactor to capture the chemical energy present in those streams. This captured energy is then used to generate steam.

Stream S212 enters the process section from section 200 and carries the flue gas coming out of the coke combustion reactor. This stream enters the process section at 900 °C and enters heat exchanger HX-401 to heat the fluidization medium for the BFCC riser, stream S311. The combustion flue gas stream is still hot coming out of the heat exchanger and is used in HX-405
to generate 10,000 kg/hr at 179 bar and 765 °C. The flue gas is then sent to the combustor R-401 to provide oxygen to be used in the combustion of the hydrocarbon side streams.

The fluidization stream, now heated to 600 °C, is split so that the required fluidization flow rate is achieved in stream S216. This stream is also combined with a nitrogen stream and flows through the gas-fired heater H-401. The fluidization stream is mixed with the nitrogen stream so that at startup there is a high enough flow rate in the BFCC riser to fluidize the biomass and catalyst. At steady state, no nitrogen should be needed to supplement the fluidization stream. The heater is also installed for startup purposes. The heater will raise the temperature of the nitrogen fluidization stream at startup when there will be no recycling of the BFCC volatile products. The fraction of stream S402 that is purged is used to heat the incoming nitrogen stream, again only used during startup, and to also heat the air used for drying the biomass in process section 100.

The purged fluidization medium leaves HX-403 and the remaining heat is captured in HX-404 to generate 3,200 kg/hr of steam at 480 °C. The stream contains approximately 20% by mass hydrocarbons that are then fed to the combustion reactor R-401.

The streams coming from the distillation columns in section 300, S316, S317, and S319, are all composed primarily of hydrocarbons. In total 3,110 kg/hr of hydrocarbons are sent into the combustion reactor in these streams. The chemical energy in these streams as well as the heated oxygen entering the reactor via stream S417 are able to generate 140,000 kg/hr of steam at 540 °C.
5.6 Process Section 500: Electricity Generation

In this process section, the steam generated in process sections 300 and 400 are sent through a turbine to generate electricity. A schematic of this section can be seen in Figure 4.6 on page 54. Streams S424, S423, S421 and S302 are combined in stream S501 to create a stream with 166,000 kg/hr of steam at 179 bar. The high pressure steam then enters a turbine where its pressure is reduced to 0.5 bar to generate 43,000 kW of electricity.
6. ENERGY BALANCES AND UTILITY REQUIREMENTS
6.1 Utility Costs Overview

The process uses three utilities: electricity, boiler-feed water, and chilled water. The annual cost for each utility is seen below in Table 6.1. The cost for all utilities sums to a total of $3,990,000. Further breakdown of each section is seen below.

<table>
<thead>
<tr>
<th>Utility</th>
<th>Annual Cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity</td>
<td>-3,499,000</td>
</tr>
<tr>
<td>Boiler-Feed Water</td>
<td>31,000</td>
</tr>
<tr>
<td>Chilled Water</td>
<td>74,000</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>(3,394,000)</strong></td>
</tr>
</tbody>
</table>

6.2 Electricity

Most of the electricity usage comes from blowers B-203 and B-401, as they account for 63% of all yearly electricity required at $6,520,000 each. Other electricity requirements come from compressors, pumps, and both distillation columns. However, the electricity generated from steam flowing through the turbine, T-501, fulfills more than the plant’s total electricity requirements, producing 43,500 kW annually, generating an excess of 6,300 kW of electricity. The revenue generated by the production of electricity in the turbine is $24 MM, using the average Louisiana electricity cost of $0.07/kWh. This results in a net positive value for electricity requirements, which generates a revenue of $3.5 MM. The breakdown for the electricity is shown below in Table 6.2.
Table 6.2 Electricity Breakdown by Equipment

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Usage (kW)</th>
<th>Cost ($/yr)</th>
<th>Usage kW/[kg/yr] BTX</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-201</td>
<td>1,537</td>
<td>852,000</td>
<td>8.84E-05</td>
</tr>
<tr>
<td>B-202</td>
<td>3,602</td>
<td>1,997,000</td>
<td>2.07E-04</td>
</tr>
<tr>
<td>B-203</td>
<td>11,763</td>
<td>6,521,000</td>
<td>6.77E-04</td>
</tr>
<tr>
<td>B-301</td>
<td>36</td>
<td>20,000</td>
<td>2.07E-06</td>
</tr>
<tr>
<td>B-401</td>
<td>11,763</td>
<td>6,521,000</td>
<td>6.77E-04</td>
</tr>
<tr>
<td>B-402</td>
<td>272</td>
<td>151,000</td>
<td>1.56E-05</td>
</tr>
<tr>
<td>C-301</td>
<td>5,393</td>
<td>2,990,000</td>
<td>3.10E-04</td>
</tr>
<tr>
<td>C-401</td>
<td>5</td>
<td>3,000</td>
<td>2.85E-07</td>
</tr>
<tr>
<td>C-402</td>
<td>292</td>
<td>162,000</td>
<td>1.68E-05</td>
</tr>
<tr>
<td>P-301</td>
<td>6</td>
<td>3,000</td>
<td>3.51E-07</td>
</tr>
<tr>
<td>P-302</td>
<td>120</td>
<td>66,000</td>
<td>6.90E-06</td>
</tr>
<tr>
<td>P-401</td>
<td>1,083</td>
<td>600,000</td>
<td>6.23E-05</td>
</tr>
<tr>
<td>Di-301</td>
<td>696</td>
<td>386,000</td>
<td>4.01E-05</td>
</tr>
<tr>
<td>Di-501</td>
<td>669</td>
<td>371,000</td>
<td>3.85E-05</td>
</tr>
<tr>
<td>T-501</td>
<td>-43,547</td>
<td>-24,142,000</td>
<td>-2.51E-03</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>-6,311</strong></td>
<td><strong>-3,499,000</strong></td>
<td><strong>-3.63E-04</strong></td>
</tr>
</tbody>
</table>

6.3 Boiler-Feed Water

Boiler-feed water was used throughout the process in the heat exchange network to generate high pressure steam for electricity generate and simultaneously cool other streams. S419 had the highest annual cost at $26,400 due to the stream having the highest flow rate out of all four streams at 55,400,000 kg/yr. The values were calculated in Table 6.3 under the assumption that the process returns 95% of the condensate from the stream so only 5% of the
stream is used for cost. The total required boiler-feed water is 65,900,000 kg/yr which translates to $31,400 assuming a cost of $4.76*10^{-5}/kg.

Table 6.3: Boiler-Feed Water Breakdown by Equipment

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Usage (kg/yr)</th>
<th>Cost ($/yr)</th>
<th>Usage kg/kg BTX</th>
</tr>
</thead>
<tbody>
<tr>
<td>S303</td>
<td>5,281,000</td>
<td>3,000</td>
<td>0.30</td>
</tr>
<tr>
<td>S415</td>
<td>1,267,000</td>
<td>1,000</td>
<td>0.07</td>
</tr>
<tr>
<td>S419</td>
<td>55,440,000</td>
<td>26,000</td>
<td>3.19</td>
</tr>
<tr>
<td>S422</td>
<td>3,960,000</td>
<td>2,000</td>
<td>0.23</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>65,949,000</strong></td>
<td><strong>31,000</strong></td>
<td><strong>3.80</strong></td>
</tr>
</tbody>
</table>

6.4 Chilled Water

Chilled water, S307, is needed for the condenser, Cn-301, in order to drop the vapor product stream, S309 to 5°C at the outlet. For this to occur, chilled water must be used at 1°C. Approximately 14,000 GJ/yr of chilled water is required for the process and using a cost of $.107/kg, this totals to $74,206 annually. These calculated costs take into account the refrigeration equipment and the electricity required to operate and maintain this low temperature. Table 6.4 shows the breakdown of the chilled water.

Table 6.4: Chilled Water Breakdown by Equipment

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Usage (GJ/yr)</th>
<th>Cost ($)</th>
<th>Usage GJ/kg BTX</th>
</tr>
</thead>
<tbody>
<tr>
<td>S307</td>
<td>14,000</td>
<td>74,000</td>
<td>.823</td>
</tr>
</tbody>
</table>
6.5 Wastewater Treatment

A wastewater treatment pond is needed to digest the trace amounts of aromatic organic compounds in the aqueous waste stream, S312, coming out of the pressurized flash vessel Fl-301. The stream contains 26,000 kilograms per year of organic molecules that will be sent to the municipal wastewater treatment facility. At a cost of $0.33 per kilogram of organic removed, the total yearly expenditures for wastewater treatment will be $8,700.
7. EQUIPMENT LIST AND UNIT DESCRIPTIONS
7.1 Section 100: Biomass Preparation

Pole Sheds: Long-term Storage

The biomass will be stored long-term in pole sheds. These pole sheds will hold 1 month of storage and be restocked monthly by procurement from a wood chip producer. Each pole shed has an area of 8,000 ft$^2$, so approximately 210 storage units will be required. This has a cost of $5,500,000. In practice, a large dome-covered area could also be used to hold 1 weeks’ worth of biomass. Daily transportation from pole sheds to the hopper will be made, but the pole sheds will be in close proximity to the plant to reduce costs and energy.

Ho-101: Short-term Storage

The hopper unit, Ho-101, provides short term storage for the wood chip biomass before it is dried and fed to grinders. Long term storage tanks hold one month’s worth of biomass feedstock whereas the hopper holds one day’s worth. The hopper has a capacity of 43,000 ft$^3$ and keeps the wood-based biomass at 25°C and an atmospheric pressure of 1.01 bar. The hopper also gravity feeds stream S101 at a flowrate of 62,200 kg/hr to the circulating fluidized bed riser, R-201, initiating the fluid catalytic cracking process. The hopper unit has a purchase cost of $77,100 and a bare module cost of $87,500. Further information about the hopper unit can be found in the specification sheet on page 98.

D-101, D-102, D-103: Feedstock Driers

Stream S101 is split off into two equal streams, each of which is fed to a dryer. There are three dryers in total, two of which operate in parallel and the third serving as an offline unit in case of malfunction and routine maintenance. The feedstock dryer units, D-101, D-102, and D-103, serve to reduce the water content in the biomass from 30% to 5% via evaporative cooling to
a warm air stream. The feedstock dryer units work using the heat supplied by these carrier gas purge streams to heat air streams, S118 and S119, transferring the heat to the biomass at a flow rate of 15,000 kg/hr with a temperature of 300°C and a pressure of 2.73 bar. The streams of biomass leaving the driers, S106 and S107, have increased in temperature, but decreased in flow rate. The outlet streams have a temperature of 175°C up from 25°C and the flow rate dropped down to 22,900 kg/hr from 31,000 kg/hr. The feedstock dryers are made of stainless steel and are direct heat-rotary, which are designed to minimize the moisture content of the biomass by bringing it in contact directly with the warm air. The total purchase cost of the feedstock dryers is $1,080,000 and the total bare module cost is $3,250,000. Further information about the dryers can be found in the specification sheet on page 99.

G-101, G-102, G-103: Feedstock Grinders

The feedstock grinders, G-101, G-102, and G-103 serve to pulverize woodchips of the biomass feed to a particle size distribution between 125-500 microns. This small size ensures that the wood chips can be fluidized by the carrier gas and cracked by the catalyst in the reactor. G-102 and G-103 operate in parallel while G-101 is offline for easy replacement and routine maintenance. The feedstock grinder is a hammer mill with a capacity of 22,900 kg/hr. A hammer mill was chosen due to its ability to pulverize material to the micron level from the constant blows of small hammers. Temperature, pressure, and flow rate are conserved passing through the feedstock grinder. Each grinder has a power requirement ranging from 50-70 kWh/ton based on the particle size distribution of 125-500 microns. The total purchase cost of G-101, G-102, and G-103 are $141,000 and a total bare module cost of $369,000. More information about the feedstock grinders can be found on the specification sheets on page 100.
The screw feeders, FS-101, FS-102, FS-103, and FS-104, act as a conveyor belt that move the biomass material to and from other pieces of equipment. FS-103 and FS-104 act in parallel while FS-102 is offline. The screw feeders are fitted with rotating helical screws that pick up the biomass and move it along the length of the screw. FS-102, FS-103, and FS-104 are used to transport dried biomass to the feedstock grinders and FS-101 is used to push ground up biomass to the riser. Flow rates, temperatures, and pressures are conserved through the screw feeder units. Screw feeders, FS-103 and FS-104, operate with a flow rate of 619 ft$^3$/hr, while FS-101 operates with a flow rate of 1240 ft$^3$/hr. The two parallel and one offline screw feeder have a total purchase cost of $16,300 and a total bare module cost of $18,400. The screw feeder that feeds to the riser, FS-101, has a purchase cost of $4,620 and a bare module cost of $5,240.

7.2 Section 200: Pyrolysis & Catalyst Regeneration

R-201: Circulating Fluidized Bed Riser

This is a vertical vessel for the fluidization of the dried, pulverized biomass from stream S115. 45,800 kg/hr of dry biomass is fed to the riser. Cracking of biomass requires that the ratio of catalyst to biomass is approximately 2:1. The ZSM-5 catalyst is continuously fed to the reactor via stream S214 at a flow rate of 99,700 kg/hr. The non-condensable products of the BFCC reaction, mostly CO, CO$_2$, and small amounts of olefins, are recycled back to act as a fluidization fluid via stream S216. The mixture of products, coke and catalyst, is lifted out of the reactor via stream S201 and proceeds towards separation units. The optimal residence time of the fluidized biomass is 2.5 seconds inside of the riser. The entrainment velocity of the fluidized biomass was calculated to be 17.35 m/sec and the required flowrate of the fluidization fluid is
required to be 35071 m/sec. This necessitates the inner diameter of the riser to be 3.5 ft and the height of the reactor to be 134 ft. The reaction takes place at low pressure, with the feed entering at 2.6 bar and leaving at atmospheric pressure at the top of the reactor. The reaction takes place at 600 °C and the temperature is assumed to stay constant throughout the riser. The heating requirement to bring the wood products up to 600 °C is .031 MMBtu/hr. This energy is supplied by the recycled carrier gas and catalyst. To handle the higher temperatures a steel vessel is used with a ceramic lining that coats the inside diameter. A riser with these specifications is estimated to have a bare module cost of $1,130,000. Details of the calculations used in determining the size of the riser can be found in Appendix A. More information about the circulating fluidized bed riser can be found on the specification sheets on page 101.

B-201: BFCC Product Centrifugal Blower

This is a centrifugal blower that moves the BFCC products from the riser into the cyclone. The blower increases the pressure of the stream 0.333 bar. It has a mass flow rate of 160,000 kg/hr and a volumetric flow rate of 3.4 x10^7 L/hr. A blower with these requirements operates at a power of 3,600 kW for a yearly utility cost of $2,000,000. The blower is estimated to have a purchase cost of $1,008,000 and a bare module cost of $1,143,000. Further details about the unit can be found in the specification sheet on page 102.

Cy-201: Coke and Catalyst Separator

This is a vertical cylindrical vessel with a conical bottom to separate coke and catalyst from the hydrocarbon BFCC products. Stream S202 carrying 191,000 kg/hr of fluidized hydrocarbons, coke and catalyst enters tangentially into a 1.21 ft. diameter, 3.65 ft. height cylinder. The solid stream containing 7,750 kg/hr of carbon coke and 67,000 kg/hr of Alumina-
Silica catalyst leaves the vessel through the bottom in stream S204. The gaseous product leaves the cyclone at a flow rate of 52,000 kg/hr through the top of the separator via stream S203. A carbon steel vessel with the specified dimensions and a thickness of .375 inches is estimated to cost $31,000. Further details about the sizing of the vessel and its specifications can be found in Appendix A and on page 103, respectively.

**R-202: Coke Combustion Reactor**

This is a vertical cylindrical vessel that exposes the coke and catalyst coming from Cy-201 via stream S206 to excess oxygen in the form of air. Stream S206 carries 107,000 kg/hr of the coke and catalyst stream to the combustor where it is mixed with 390,000 kg/hr of air. The amount of oxygen consumed is 20,800 kg/hr and the corresponding amount of CO₂ produced is 27,900 kg/hr. The energy produced by the combustion reaction is 20,200 MMBtu/hr. Oxygen is fed to the combustor in approximately 4.5 times the stoichiometric requirement. This is so that the excess air can act as a diluent and prevent the catalyst from heating to a temperature where it may lose its functionality. 498,000 kg/hr of product consisting of 5.6% CO₂, 60.2% nitrogen, 14.2% oxygen and 20.0% catalyst by mass leave the reactor via stream S209. The required size of the reactor was found by setting the residence time of the reactor to be 1 min. The long residence time is required to react all of the solid coke with the gaseous oxygen. The resulting dimensions of the reactor are 24.68 ft. tall with a 8.23 ft. inner diameter and a wall thickness of 0.563 in. A vessel of this size is estimated to have a purchase cost of $78,300 and a bare module cost of $323,000. Further information regarding the sizing of the vessel can be found in Appendix A and the specification sheet for this unit can be found on page 105.
Cy-202: Catalyst and Combustion Flue Gas Separator

A vertical cylindrical vessel with a conical bottom used to separate catalyst from the gaseous components resulting from the combustion of the coke. The product leaves at 398,000 kg/hr of product consisting of 5.61% CO₂, 60.2% nitrogen, 14.2% oxygen and 20.0% catalyst by mass enters the cyclone tangentially via stream S210. The solid stream containing 99,000 kg/hr of carbon coke and leaves the vessel through the bottom. The gaseous product leaves the separator with a flow rate of 398,000 kg/hr through the top of the cyclone with a mass fraction of 0.07 carbon dioxide, 0.75 nitrogen and 0.18 oxygen. The vessel will have a height of 49.4 ft. and a diameter of 16.5 ft. A carbon steel vessel with the specified dimensions and a thickness of 0.625 inches is estimated to have a purchase cost of $212,000 and a bare module cost of $884,000. Further details about the sizing of the vessel and its specifications can be found in Appendix A and on page 107, respectively.

7.3 Section 300: Product Separation

HX-301: BFCC Product and Water Heat Exchanger

Fixed head shell and tube heat exchanger that cools the BFCC gaseous products coming from Cy-201 using water to generate steam. Stream 301, containing 52,000 kg/hr of the products from the BFCC reaction and coming from process section 200 via stream S301, enters the tube side of the reactor at 600 °C and atmospheric pressure. 13,000 kg/hr of boiler water enters the shell side of the exchanger at 25 °C and 179 bar in stream S303. The cooled gases leave the exchanger via stream S304 at 80 °C, transferring 38 MMBtu/hr of energy to the water. The water leaves the shell side via stream S302 at 411 °C. The heat exchanger has a tube length of 20 ft and a surface area of 1750 square feet and is made of stainless steel. A heat exchanger with these
specifications is estimated to have a purchase cost of $19,900 and a bare module cost of $107,000. Further details about this heat exchanger can be found on its specification sheet of page 108.

**C-301: BFCC Product Centrifugal Compressor**

Compressor that brings the BFCC gaseous products to high pressure for entry to the flash drum. The cooled BFCC products enter the compressor via stream S403 at 80 °C and atmospheric pressure with a flow rate of 52,000 kg/hr. Stream S305 leaves the compressor at 9 bar and 326 °C. The power requirement for this compressor is 5,400 kW which results in a yearly utility cost of $3,000,000. A compressor with these size and power requirements is estimated to have a purchase cost of $2,400,000 and a bare module cost of $6,250,000. Further details about this compressor can be found in its specification sheet on page 109.

**Cn-301: BFCC Product Condenser**

Series of four shell and tube heat exchanger that condenses the high pressure BFCC product stream in preparation for product separation. Stream S305 enters the tube side of the heat exchanger at 326 °C and 9 bar. All of the 52,000 kg/hr of BFCC product mixture enter the heat exchanger as a vapor. This hot stream leaves the exchanger at 5 °C via stream S309 to enter a flash separation vessel. The vapor fraction of the product stream leaving the exchanger is .728. The shell side of the first two heat exchangers contains 40,000 kg/hr of process water which leaves the heat exchangers at 100 °C. The product is cooled to below ambient temperatures using two additional heat exchangers using 15,000 kg/hr of chilled water which leaves at 22°C. Each exchanger has a surface area of 9,000 square feet and are estimated to have a purchase cost of
$64,000 and a bare module cost of $247,000. This results in the unit costing an estimated $990,000. Further details about this unit can be found in its specification sheet on page 111.

**P-301: Centrifugal Pump for Chilled Water**

Pump used to pressurize the chilled water in stream S307. The pump elevates the pressure of the chilled water to 4.11 bar from atmospheric pressure. The pump produces 106 feet of head and has a volumetric flow rate of 55,000 kg/hr. The pump uses 6 kW of electricity, resulting in a yearly utility cost of $3,300. A pump with these specification is estimated to have a purchase cost of $4,570 and a bare module cost of $16,700. Further details of this unit can be found on the specification sheet on page 110.

**Fl-301: Vapor-Liquid-Liquid Flash Vessel**

Cylindrical flash vessel for separating the volatile, aqueous and organic phases of the BFCC product. The BFCC product mix enters the flash drum with a flow rate of 52,000 kg/hr via stream S309 at 5 °C and 9 bar. The flash vessel exists at these same conditions and allows for the aqueous, organic, and volatile streams to separate. The volatile stream exits the top of the reactor via stream S310. This stream has a flow rate of 40,000 kg/hr and consists of 59% carbon monoxide, 28% carbon dioxide, 6% methane, and 4% ethylene by mass. The remainder consists of trace amounts aromatic compounds. The aqueous components of the BFCC reaction leave the bottom of the vessel via stream S312 towards the wastewater treatment. This stream has a flow rate of 9,000 kg/hr and is made up of 99.9% water with the remainder being phenol and trace amounts of aromatics. The organic stream leaves the vessel via stream S313 with a flow rate of 3,000 kg/hr. The stream is made up of 20% benzene, 29% toluene, 13% xylenes, 5% styrene and
14% naphthalene with trace amounts of water, olefins, and carbon dioxide. The vessel is a vertical cylinder with a diameter of 3.1 meters and a height of 18.13. The vessel has a wall thickness of .392 inches in order to withstand the higher pressure. A stainless steel vessel with these dimensions is estimated to have a purchase cost of $20,000 and a bare module cost of $83,000. More information regarding the sizing of this vessel can be found in Appendix A and further details about the unit can be found in the specification sheet on page 112.

**B-301: Volatile Product Centrifugal Blower**

Centrifugal blower used to move the volatile products from the flash vessel in stream S310 to a combustion vessel reactor. The blower increases the pressure of the stream 0.333 bar. It has a mass flow rate of 40,000 kg/hr and a volumetric flow rate of 3,550,000 L/hr. A blower with these requirements operates at a power of 36 kW for a yearly utility cost of $20,000. The blower is estimated to have a purchase cost of $220,000 and a bare module cost of $252,000. Further details about the unit can be found in the specification sheet on page 113.

**P-302: Centrifugal Pump for Aqueous BFCC Products**

Pump used to pressurize the aqueous products leaving the flash vessel in stream S312. The pump elevates the stream by 1.7 bar for transportation to a wastewater treatment facility. The pump produces 59 ft. of head and has mass and volumetric flow rates of 9,000 kg/hr and 9,230 L/hr respectively. A pump with these specifications consumes 0.5 kW and has an annual utility cost of $227. The pump will be made of cast iron and it is estimated that the pump have a purchase cost of $3,270 and a bare module cost of $12,200. Further details about the unit can be found in the specification sheet on page 114.
Distillation column used to remove high-boiling aromatic compounds from stream S309. The column utilizes differences in boiling points between high-boiling aromatic compounds such as naphthalene indene and phenol and lower-boiling aromatic compounds benzene, toluene, the xylenes and styrene. The column includes 27 sieve stages with a spacing of 1.5 ft., a 10 ft. sump and an overhead space of 4 feet. This results in a total vertical height of 54 ft. The diameter necessary for the column was calculated so that the internal velocity is 80% of the flooding velocity using the average density and flow rate throughout the column of both the vapor and liquid components. It was calculated that the necessary diameter of the column be 3.16 ft. 3,000 kg/hr of the aromatic compound mixture enters the column via stream S313 at 5 °C and 9 bar.

A vapor product stream at 3,980 kg/hr, 180 °C and 4.9 bar enter the condenser from the top stage of the distillation column. The stream is cooled to 30 °C using 25 °C process water and transfers 2.37 MMBtu/hr of energy to the cooling water.

The cooled products are transferred to a reflux accumulator so that the non-condensable olefins and paraffins can be separated from the valuable aromatic products. 24.5 kg/hr of the non-condensable products leave the reflux accumulator via stream S315 to head to a combustor to capture any heating value in the stream. The condensed aromatic stream leaves the reflux accumulator with a flow rate of 3,950 kg/hr. This stream is split so that 2,310 kg/hr of the aromatics leave the unit via stream S316 and the remainder head back into the column as reflux, with a reflux ratio of 0.713. The reflux accumulator is sized so that the overhead product can have a residence time of five minutes, using only half of the available volume. The vessel was calculated to need a 6 ft. length and a 2.8 ft. diameter.
At the bottom of the column, 690 kg/hr of the heavy aromatic compounds leave the column via stream S17. The column has a boilup ratio of 14.6 and thus 8,900 kg/hr of the bottoms product is vaporized and sent back into the distillation column. The energy needed to vaporize the stream is 2.86 MMBtu/hr and is supplied by a gas fired kettle reboiler. A carbon steel distillation column with these ancillary components is estimated to have a purchase cost of $86,400 and a bare module cost of $359,000. Further details about this unit can be found on the specification sheet on page 115. This unit was sized using parameters found in Seider et al.[30].

Di-302: Distillation Column for Removal of Phenol from BTX with Reboiler and Condenser

Vertical Distillation designed to remove phenol from the non-oxygenated aromatic compounds in stream S316.2310 kg/hr of aromatic products from Di-301 enter Di-302 at 30 °C and 4.7 bar. The column has 15 stages, each separated by 1.5 ft., a 10 ft. sump section, and a 4 ft. overhead space for a total of 35 ft. The diameter is 3.16 ft. 3,740 kg/hr leave the top stage as a vapor and enter the tube side of a shell and tube heat exchanger at 173 °C. The vapor product is cooled to 25 °C using process water. The required heat transfer to achieve this level of cooling is 2.28 MMBtu/hr. The cooled vapor product is completely liquid and is at its bubble point. The overhead product is then enters a 5.5 ft. by 2.5 ft. reflux accumulator where it is split into two streams. 2,200 kg/hr leave the reflux accumulator as the final product in stream S318. With a reflux ratio of .75, 1640 kg/hr reenter the distillation column as liquid reflux. The overhead product in stream S318 consists of 27% benzene, 40% toluene, 19% benzene, 6% styrene 2% ethylbenzene 1% phenol and the remainder large aromatic compounds.

At the bottom stage of the column, 6,210 kg/hr leave the column as a liquid. 6,100 kg/hr of this stream is evaporated using 2.27 MMBtu/hr and a cast iron kettle reboiler. 120kg/hr is split
off as a bottoms product and heads towards the combustor via stream S319 and contains 71% phenol, 6.3% indene, and 22% benzofuran.

A distillation column plus the ancillary condenser, reboiler and reflux accumulator has an estimated purchase cost of $67,000 dollars and a bare module cost of $281,000. Further details regarding the specification of this unit can be seen on the specification page on page 116. This unit was sized using parameters found in Seider et al. [30].

7.4 Section 400: Heat Integration

**B-401: Blower**

B-401 was used specifically to transport the volatile stream, S211, to heat exchanger, HX-401. Mass is conserved through this centrifugal blower, but there are temperature increases as well as minor pressure increases. The outlet stream, S401, has a temperature of 907°C up from 700°C and a pressure of 2.03 bar up from 1 bar. B-401 is made of a cast iron/carbon-steel material with a power requirement of 40,000 hp and will consume about 256 kW of electricity. Two of these blowers are needed for this transport and each has a purchase cost of $9,230,000 and the total bare module cost is $20,940,000. The specification on page 117 has more information about the blower.

**B-402: Blower**

Blower, B-402, is designed to transport air for the biomass drying step. There is also a temperature and pressure increase similar to B-401. The outlet stream, S410, has a temperature of 137°C up from 25°C and a pressure of 2.74 bar up from 1.01 bar. B-402 has a volumetric capacity of 14,900 ft³/min and is made of the same material as the other blower, B-401, as well
as have a similar electricity consumption rate at 272 kW. It has a purchase cost of $132,000 and a bare module cost of $150,000. Page 122 has more information about the blower including the specification sheet.

**HX-401: Heat Exchanger**

Heat exchanger, HX-401, was designed to cool down the recycled volatile stream, S416, that will be used as carrier gas in the circulating fluidized bed of the process. Mass and pressure remained unchanged through the heat exchanger, however there were obvious temperature changes. On the shell side stream S402 was raised to 600°C up from 28°C, while on the tube side the volatile stream from the cyclone, S416, was decreased to 938°C down from 1000°C. HX-401 and all other heat exchangers are carbon steel shell and tube heat exchangers with a fixed head operating with counter-current flow. HX-401 uses tube lengths of 20 ft with a surface area of 167 ft$^2$ and a heat duty of 28 MMBtu/hr. Its utility is from the volatile stream which comes from the catalyst regenerator at 39,900 kg/hr. Its purchase cost is $9,420 and its bare module cost is $34,100. More information on this heat exchanger can be found on its specification sheet on page 118.

**HX-402: Heat Exchanger**

Heat exchanger, HX-402, was designed to use the heat from the carrier gas purge stream, S403, and heat up the nitrogen gas stream which then travels to the circulating fluidized catalytic reactor. On the shell side, the nitrogen stream is being heated up to 590°C up from 179°C and on the tube side, the purge stream is dropping in temperature to 599°C down from 600°C. HX-402 has a surface area of 1.44 ft$^2$ with a heat duty of 42.5 MBtu/hr. Its utility is only from the hot purge stream flowing at 26,200 kg/hr. Its purchase cost is $15,800 and its bare
module cost is $61,200. More information on this heat exchanger can be found on its specification sheet on page 120.

**HX-403: Heat Exchanger**

Heat exchanger, HX-403, was designed to transfer heat from the recently compressed carrier gas purge stream, S411, to the air stream, S116, to dry the wood biomass in the dryer unit. On the shell side, the air stream, S116, rises in temperature to 300°C from initially 136°C, while on the tube side, the purge stream, S411, drops in temperature to 491°C from initially 623°C. HX-403 has a surface area of 52.3 ft² with a heat duty of 5 MBtu/hr. Its utility is from the hot purge stream as well flowing at 26,200 kg/hr. Its purchase cost is $9,770 and its bare module cost is $33,400. More information on this heat exchanger can be found on its specification sheet on page 123.

**C-401: Vapor Compressor**

C-401 was designed to transport nitrogen carrier gas for preheating before entering the circulating fluidized bed riser. Mass was conserved throughout the compressor, however the temperature and pressure changed significantly. The outlet stream, S405, has a temperature of 179°C up from 25°C and a pressure of 3.77 bar up from 1.01 bar. C-401 has a power requirement of 6.64 hp and consumes 5 kW of electricity for its utility cost. The purchase cost is $13,300 and the bare module cost is $34,700. More information on the compressor can be found on its specification sheet on page 119.
C-402: Vapor Compressor

C-402 was designed to transport the carrier gas purge stream in order to heat up the air being used for drying the biomass. The outlet stream, S408, rose to 623°C from an initial value of 599°C and the pressure rose to 14.2 bar from initially at 12.4 bar. Its power requirement is 392 hp and its utility cost is 292 kW of electricity. The purchase cost is $233,000 and the bare module cost is $607,000. More information on the compressor can be found on its specification sheet on page 121.

P-401: Pump

Pump, P-401, was used to transport cooling water to a low pressure steam economizer, HX-404. The outlet stream, S413, has a small rise in temperature and significant increase in pressure. The temperature rises to 26°C up from 25°C and the pressure rises to 179 bar up from 1.01 bar. The pump was modeled as a centrifugal compressor made of cast iron/carbon-steel. It has a power requirement of 1,450 hp and consumes 1,080 kW of electricity for utilities. It has a purchase cost of $4,950 and a bare module cost of $18,500. For more information on the pump and its specification sheet, refer to page 124.

HX-404: High Pressure Steam Economizer

HX-404 was designed to cool down flue gases produced from catalytic regeneration and co-produce low pressure steam. Mass and pressure is conserved throughout the economizer. On the shell side cool water enters in as a liquid at 26°C and exits at 480°C as steam, while on the tube side, the flue gas comes in at 491°C and exits at 193°C. HX-404 has a surface area of 642 ft² with a heat duty of 10 MBtu/hr. The purchase cost is $12,700 and the bare module cost is
$70,400. More information on this steam economizer can be found on its specification sheet on page 125.

**HX-405: High Pressure Steam Economizer**

HX-405 was designed to similarly cool down flue gases from the catalytic regenerator and co-generate low pressure steam. On the shell side, liquid water, S422, at 26°C is raised to steam, S423, at 765°C, while on the tube side the flue gas, S416, at 844°C is lowered to 759°C in S417. HX-405 has a surface area of 288 ft² with a heat duty of 82.7 MBtu/hr. It has a purchase cost of $10,200 and a bare module cost of $55,100. More information on this steam economizer can be found on its specification sheet on page 126.

**HX-406: High Pressure Steam Economizer**

Lastly, HX-406 was designed to cool down flue gases from the waste heat boiler and co-generate low pressure steam. On the shell side liquid water, S419, enters at 25°C and exits at 200°C in S421, while on the tube side flue gas, S418, enters at 1072°C and exits at 95°C in S420. HX-406 has a surface area of 7,340 ft² with a heat duty of 450 MBtu/hr. Its purchase cost is $53,700 and a bare module cost of $298,000. More information on this steam economizer can be found on its specification sheet on page 128.

**R-401: Combustor**

The combustor reactor, R-401, was designed to combust purged volatile streams for their heating value. For this specific combustor, there are four inlets, S417, S414, S316, and S317, and one outlet, S418. The first inlet, S417, is a vapor stream composed of air and carbon dioxide and is
fed in at 398,000 kg/hr at 759°C and 2.03 bar. The next inlet, S414, is a vapor stream composed of flue gases produced from catalytic regeneration. The breakdown of the stream is 60% carbon dioxide, 28% carbon monoxide and 6% methane and it enters at 26,200 kg/hr with a temperature of 193°C and a pressure of 14.2 bar. S316 is another volatile vapor stream that is composed of mainly carbon monoxide at 63% and carbon dioxide at 16%. The stream enters at 30°C and a pressure of 4.76 bar with a flow rate of 24.6 kg/hr. The last inlet, S317, is the high boil liquid stream from the distillation column, Di-301. It’s composed of 63% naphthalene, 30% indene, and 5% phenol by mass. It enters with a flow rate of 690 kg/hr at 314°C and 8.5 bar. The outlet vapor stream, S418, is composed mainly of air, carbon monoxide, carbon dioxide and water, the typical product in a combustion reaction. The stream leaves the combustor at 426,000 kg/hr at 1072°C and 1.01 bar. The combustor, R-401, was modeled as a vertical vessel with stainless steel and ceramic lined exterior to prevent heat from escaping. It has a height of 37.6 ft. with a diameter of 12.5 ft. with a heat duty of 478 MMBtu/hr. The purchase cost is $145,000 with a bare module cost of $603,000. More information about the combustor including its specification sheet can be found on page 127.

7.5 Section 500: Electricity Generation

T-501: Steam Turbine

Isentropic power-recovery turbine used to generate steam from excess heat captured in process sections 200 and 300. Streams S424, S423, S421 and S302 are combined in stream S501 to create a stream with 166,000 kg/hr of steam at 179 bar. The high pressure steam then enters a turbine where its pressure is reduced to .5 bar against a vacuum to generate 43,000 kW of
electricity. The turbine is designed as a gas expander with a vacuum discharge with 8000 hp extracted. The purchase cost is $13,800,000 and the bare module cost is $15,700,000. More information about the turbine, including its specification sheet, can be found on page 129.
8. SPECIFICATION SHEETS
8.1 Section 100: Biomass Preparation

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<thead>
<tr>
<th><strong>Hopper</strong></th>
<th></th>
</tr>
</thead>
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<tr>
<td><strong>Identification:</strong></td>
<td><strong>Item</strong> Hopper bin</td>
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<tr>
<td>Item No.</td>
<td>Ho-101</td>
</tr>
<tr>
<td>No. Required</td>
<td>1</td>
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</tbody>
</table>

| **Function:** | To transport wet biomass from long term storage to provide daily input capacity for plant; gravity fed |
| **Operation:** | Semi-Continuous |

| **Performance of Unit** |  |
| **Inlet 1** | **Inlet 2** |
| Stream I.D. | From Long Term Storage | S101 |
| Temperature (°C) | 25 | 25 |
| Pressure (bar) | 1.01 | 1.01 |
| Phase | Solid | Solid |
| Mass Flow Rate (kg/hr) | Wood: 62,180.00 | 43,526.00 |
| | Water: 18,654.00 | 18,654.00 |

| **Design Data:** | **Type:** Bin |
| **Capacity:** | 43,002.2 ft³ |

| **Utilities:** | None |

| **Cost Information:** | **Purchase Cost:** $77,140.17 |
| **Total Bare Module Cost:** | $87,476.95 |
### Dryer

**Identification:** Item Evaporative Cooler
Item No. D-101
No. Required 3

**Function:** To reduce moisture content of biomass from 30% to 5%

**Operation:** Continuous

#### Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Outlet 1</th>
<th>Outlet 2</th>
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<td>S102</td>
<td>S117</td>
<td>S105</td>
<td>S120</td>
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<tr>
<td>Temperature (°C)</td>
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<td>175</td>
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<tr>
<td>Pressure (bar)</td>
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<td>1.01</td>
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<td>Phase</td>
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<td>Solid/Liquid</td>
<td>Vapor</td>
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<td>Wood</td>
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<tr>
<td>Water</td>
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<td>2,290.84</td>
<td>16,363.20</td>
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**Design Data:**
- Type: Direct Heat-Rotary
- Material: Stainless Steel
- Dimensions: Area: 870 m²

**Utilities:**
Heat supplied by carrier gas purge stream: 26,1923 kg/hr at 598.83 °C and 14.6 bar

**Cost Information:**
- Purchase cost per unit: $463,328.58
- Bare Module Cost per unit: $1,082,354.10
- Total Bare Module Cost: $3,247,062.29
### Grinder

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**Function:** To reduce size of woodships to obtain a particle size distribution between 125-500 micron

**Operation:** Continuous

### Performance of Unit

<table>
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<tr>
<th></th>
<th>Inlet 1</th>
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</tr>
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<tbody>
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<td>1.01</td>
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<td>Solid</td>
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<tr>
<td>Water</td>
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</table>

**Design Data:**
- Type: Hammer Mill
- Capacity: 25.25 dry ton/hr

**Utilities:**
- 50-70 kWh/ton to grind woodships to a particle size distribution of 125-500 microns

**Cost Information:**
- Purchase Cost per unit: $47,157.14
- Bare Module Cost per unit: $122,955.26
- Total Bare Module Cost: $368,985.77
8.2 Section 200: Pyrolysis & Catalyst Regeneration

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<td>No. Required</td>
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<tr>
<td><strong>Function:</strong></td>
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<tr>
<td><strong>Operation:</strong></td>
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<table>
<thead>
<tr>
<th>Performance of Unit</th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Inlet 3</th>
<th>Outlet</th>
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<td>S214</td>
<td>S216</td>
<td>S201</td>
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<td>0.95</td>
<td>185.32</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>-</td>
<td>-</td>
<td>1.01</td>
<td>185.38</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>-</td>
<td>-</td>
<td>0.23</td>
<td>58.62</td>
</tr>
<tr>
<td>Water</td>
<td>2,290.84</td>
<td>-</td>
<td>5.47</td>
<td>9,043.33</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Design Data:</th>
<th>Type: Vertical Vessel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material:</td>
<td>Stainless Steel with Ceramic Lined Exterior</td>
</tr>
<tr>
<td>Dimensions:</td>
<td>Diameter 12.52 ft</td>
</tr>
<tr>
<td></td>
<td>Height 37.56 ft</td>
</tr>
<tr>
<td>Geometry: Tall, thin pyrolysis section with wider disengagement section above</td>
<td></td>
</tr>
<tr>
<td>Heat Duty: 203,726 MMBtu/hr</td>
<td></td>
</tr>
</tbody>
</table>

| Utilities:          | Fired heater will provide heat to reach 600 °C upon startup. Heat from catalytic regeneration will maintain steady-state temperature. |

<table>
<thead>
<tr>
<th>Cost Information:</th>
<th>Purchase Cost: $271,058.49</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Total Bare Module Cost: $1,127,603.30</td>
</tr>
</tbody>
</table>
# Blower

**Identification:**
- **Item:** Centrifugal Blower
- **Item No.:** B-201
- **No. Required:** 1

**Function:** To increase the pressure of the vapor product stream from the reactor entering the solid/vapor cyclone.

**Operation:** Continuous

<table>
<thead>
<tr>
<th><strong>Stream I.D.</strong></th>
<th><strong>Inlet</strong></th>
<th><strong>Outlet</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Temperature (°C)</strong></td>
<td>653</td>
<td>705</td>
</tr>
<tr>
<td><strong>Pressure (bar)</strong></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td><strong>Phase</strong></td>
<td>Solid/Vapor</td>
<td>Solid/Vapor</td>
</tr>
<tr>
<td><strong>Mass Flow Rate (kg/hr)</strong></td>
<td>159,227.40</td>
<td>159,227.40</td>
</tr>
</tbody>
</table>

**Mass Flow Rate (kg/hr):**
- **Aluminum-Silicate-Kyanite:** 99,590.80
- **Benzene:** 744.96
- **Benzoic acid:** 54.76
- **Butadiene:** 166.85
- **Butene:** 66.97
- **Carbon Dioxide:** 23,626.40
- **Carbon Monoxide:** 11,393.60
- **Cellobiose:** 31,469.30
- **Coke:** 7,635.48
- **Diphenyl ether:** 6,028.35
- **Ethylbenzene:** 37.09
- **Ethylene:** 1,508.74
- **Guaiacol:** 6,028.35
- **Indene:** 212.30
- **Methane:** 2,314.63
- **Naphthalene:** 436.33
- **Nitrogen:** 152.37
- **Phenol:** 145.35
- **Propylene:** 602.97
- **Styrene:** 133.29
- **Toluene:** 932.41
- **m-Xylene:** 185.32
- **p-Xylene:** 185.38
- **o-Xylene:** 58.62
- **Water:** 9,043.33

**Design Data:**
- **Type:** Centrifugal Compressor
- **Material:** Cast Iron/Carbon-Steel
- **Specific Heat Ratio:** 1.4
- **Volumetric Capacity:** 84,315 ft³/min

**Utilities:**
- **Electricity at 1,537 kW**

**Cost Information:**
- **Purchase Cost:** $515,254.98
- **Total Bare Module Cost:** $584,299.15
**Cyclone**

<table>
<thead>
<tr>
<th><strong>Identification:</strong></th>
<th><strong>Item:</strong></th>
<th>Concical Head Cyclone</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Item No.:</strong></td>
<td>Cy-201</td>
<td></td>
</tr>
<tr>
<td><strong>No. Required:</strong></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Function:** To separate pyrolysis vapor products from coke, ash, and reaction catalyst.

**Operation:** Continuous

<table>
<thead>
<tr>
<th><strong>Performance of Unit</strong></th>
<th><strong>Inlet 1</strong></th>
<th><strong>Outlet 1</strong></th>
<th><strong>Outlet 2</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S202</td>
<td>S203</td>
<td>S204</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>653</td>
<td>600</td>
<td>600</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>2.03</td>
<td>1.01</td>
<td>1.01</td>
</tr>
<tr>
<td>Phase</td>
<td>Solid/Vapor</td>
<td>Vapor</td>
<td>Solid</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>59,636.60</td>
<td>52,001.10</td>
<td>7,635.48</td>
</tr>
<tr>
<td>Aluminum-Silicate-Kyanite</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Benzene</td>
<td>744.96</td>
<td>744.96</td>
<td>-</td>
</tr>
<tr>
<td>Benzo-furan</td>
<td>54.76</td>
<td>54.76</td>
<td>-</td>
</tr>
<tr>
<td>Butadiene</td>
<td>166.85</td>
<td>166.85</td>
<td>-</td>
</tr>
<tr>
<td>Butene</td>
<td>66.38</td>
<td>66.38</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>23,626.40</td>
<td>23,626.40</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>11,393.60</td>
<td>11,393.60</td>
<td>-</td>
</tr>
<tr>
<td>Cello-biose</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Coke</td>
<td>7,635.48</td>
<td>-</td>
<td>7,635.48</td>
</tr>
<tr>
<td>Diphenyl ether</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>37.09</td>
<td>37.09</td>
<td>-</td>
</tr>
<tr>
<td>Ethylene</td>
<td>1,508.74</td>
<td>1,508.74</td>
<td>-</td>
</tr>
<tr>
<td>Guaiacol</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Indene</td>
<td>212.30</td>
<td>212.30</td>
<td>-</td>
</tr>
<tr>
<td>Methane</td>
<td>2,314.63</td>
<td>2,314.63</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>436.33</td>
<td>436.33</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>152.37</td>
<td>152.37</td>
<td>-</td>
</tr>
<tr>
<td>Phenol</td>
<td>145.35</td>
<td>145.35</td>
<td>-</td>
</tr>
<tr>
<td>Propylene</td>
<td>602.97</td>
<td>602.97</td>
<td>-</td>
</tr>
<tr>
<td>Styrene</td>
<td>133.29</td>
<td>133.29</td>
<td>-</td>
</tr>
<tr>
<td>Toluene</td>
<td>932.41</td>
<td>932.41</td>
<td>-</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>185.32</td>
<td>185.32</td>
<td>-</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>185.38</td>
<td>185.38</td>
<td>-</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>58.62</td>
<td>58.62</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>9,043.33</td>
<td>9,043.33</td>
<td>-</td>
</tr>
</tbody>
</table>

**Design Data:**

<table>
<thead>
<tr>
<th><strong>Type:</strong></th>
<th>Vertical Vessel</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Material:</strong></td>
<td>Carbon Steel</td>
</tr>
<tr>
<td><strong>Dimensions:</strong></td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>1.21 ft</td>
</tr>
<tr>
<td>Height</td>
<td>3.65 ft</td>
</tr>
<tr>
<td><strong>Geometry:</strong></td>
<td>Cylinder with conical head</td>
</tr>
</tbody>
</table>

**Utilities:** None

**Cost Information**

<table>
<thead>
<tr>
<th><strong>Purchase Cost:</strong></th>
<th>$7,442.46</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total Bare Module Cost:</strong></td>
<td>$30,960.65</td>
</tr>
</tbody>
</table>
### Blower

<table>
<thead>
<tr>
<th><strong>Identification:</strong></th>
<th>Item</th>
<th>Centrifugal Blower</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>B-202</td>
<td></td>
</tr>
<tr>
<td>No. Required</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Function:</strong></th>
<th>To increase the pressure of the air required for catalyst regeneration</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th><strong>Operation:</strong></th>
<th>Continuous</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th><strong>Performance of Unit</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inlet</strong></td>
</tr>
<tr>
<td>Stream I.D.</td>
</tr>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Phase</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
</tr>
<tr>
<td>Nitrogen</td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Design Data:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Type:</td>
</tr>
<tr>
<td>Material:</td>
</tr>
<tr>
<td>Specific Heat Ratio:</td>
</tr>
<tr>
<td>Volumetric Capacity:</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Utilities:</strong></th>
<th>Electricity at 3,602 kW</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th><strong>Cost Information:</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchase Cost:</td>
</tr>
<tr>
<td>Total Bare Module Cost:</td>
</tr>
</tbody>
</table>
### Reactor

**Identification:** Item Combustor  
**Item No.** R-202  
**No. Required** 1

**Function:** To burn off coke adhered to the catalyst, thereby regenerating it.

**Operation:** Continuous

<table>
<thead>
<tr>
<th>Performance of Unit</th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S206</td>
<td>S208</td>
<td>S209</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>600</td>
<td>137</td>
<td>600</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.01</td>
<td>2.72</td>
<td>1</td>
</tr>
<tr>
<td>Phase</td>
<td>Solid</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>7,626.54</td>
<td>390,859.00</td>
<td>398,486.00</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>-</td>
<td>-</td>
<td>27,944.60</td>
</tr>
<tr>
<td>Coke</td>
<td>7,626.54</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>-</td>
<td>299,821.00</td>
<td>299,821.00</td>
</tr>
<tr>
<td>Oxygen</td>
<td>-</td>
<td>91,037.70</td>
<td>70,719.60</td>
</tr>
</tbody>
</table>

**Design Data:**  
**Type:** Vertical Vessel  
**Material:** Carbon Steel  
**Dimensions:**  
- Diameter: 8.23 ft  
- Height: 24.68 ft

**Utilities:** Electricity at 15,932.3 kW

**Cost Information:**  
**Purchase Cost:** $78,297.57  
**Total Bare Module Cost:** $325,717.87

---

105
<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item</th>
<th>Centrifugal Blower</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td></td>
<td>B-203</td>
</tr>
<tr>
<td>No. Required</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Function:** To transport flue gases and regenerated catalyst from combustor to solid/vapor cyclone.

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S209</td>
<td>S210</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>700</td>
<td>861</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1</td>
<td>2.03</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>497,959.50</td>
<td>497,959.50</td>
</tr>
<tr>
<td>Aluminum-Silicate-Kyanite</td>
<td>99,474.30</td>
<td>99,474.30</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>27,944.60</td>
<td>27,944.60</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>299,821.00</td>
<td>299,821.00</td>
</tr>
<tr>
<td>Oxygen</td>
<td>70,719.60</td>
<td>70,719.60</td>
</tr>
</tbody>
</table>

### Design Data:
- **Type:** Centrifugal Blower
- **Material:** Cast Iron/Carbon-Steel
- **Specific Heat Ratio:** 1.4
- **Volumetric Capacity:** 645,397 ft³/min

### Utilities:
- **Electricity at 11,663 kW**

### Cost Information:
- **Combined Purchase Cost:** $2,574,123.62
- **Total Bare Module Cost/unit:** $2,919,056.18
<table>
<thead>
<tr>
<th>Cyclone</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Function:</strong></td>
</tr>
<tr>
<td><strong>Operation:</strong></td>
</tr>
<tr>
<td><strong>Performance of Unit</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Stream I.D.</td>
</tr>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Phase</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
</tr>
<tr>
<td>Aluminum-Silicate-Kyanite</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
</tr>
<tr>
<td>Nitrogen</td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
<tr>
<td><strong>Design Specifications</strong></td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td><strong>Cost Information</strong></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>
### 8.3 Section 300: Product Separation

#### Heat Exchanger

<table>
<thead>
<tr>
<th>Identification: Item</th>
<th>Fixed Head Shell and Tube Heat Exchanger</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>HX-301</td>
</tr>
<tr>
<td>No. Required</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function:** To cool vapor product in preparation for extraction of valuable products

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream I.D.</strong></td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td>S303</td>
<td>S302</td>
<td>S301</td>
</tr>
<tr>
<td><strong>Temperature (°C)</strong></td>
<td>25</td>
<td>412</td>
</tr>
<tr>
<td><strong>Pressure (bar)</strong></td>
<td>179</td>
<td>179</td>
</tr>
<tr>
<td><strong>Phase</strong></td>
<td>Liquid</td>
<td>Vapor</td>
</tr>
<tr>
<td><strong>Mass Flow Rate (kg/hr)</strong></td>
<td>13,337.00</td>
<td>13,337.00</td>
</tr>
<tr>
<td>Benzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butadiene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Indene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Methane</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Phenol</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Propylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Styrene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Toluene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>13,337.00</td>
<td>13,337.00</td>
</tr>
</tbody>
</table>

### Design Data:

- **Type:** Shell & Tube, Fixed Head
- **Flow Type:** Counter-Current
- **Material:** Carbon Steel
- **Tube Length:** 20 ft
- **Dimensions:** Surface Area: 1,746 ft²
- **Heat Duty:** 38 MMBtu/hr

### Utilities:

- Cooling water at ambient temperature, 13,337 kg/hr

### Cost Information:

- **Purchase Cost:** $19,914.75
- **Total Bare Module Cost:** $107,574.76
**Identification:** Centrifugal Compressor  
**Item No.:** C-301  
**No. Required:** 1

**Function:** To transport vapor product stream from the circulating fluidized bed riser to the product separation block

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>S304</td>
<td>52,029.30</td>
<td>52,029.30</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>80</td>
<td>327</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.01</td>
<td>9</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>753.68</td>
<td>753.68</td>
</tr>
<tr>
<td>Benzene</td>
<td>54.77</td>
<td>54.77</td>
</tr>
<tr>
<td>Butadiene</td>
<td>168.64</td>
<td>168.64</td>
</tr>
<tr>
<td>Butene</td>
<td>67.00</td>
<td>67.00</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>27.12</td>
<td>27.12</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>11,401.90</td>
<td>11,401.90</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>37.14</td>
<td>37.14</td>
</tr>
<tr>
<td>Ethylene</td>
<td>1,509.54</td>
<td>1,509.54</td>
</tr>
<tr>
<td>Indene</td>
<td>212.32</td>
<td>212.32</td>
</tr>
<tr>
<td>Methane</td>
<td>2,314.85</td>
<td>2,314.85</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>436.34</td>
<td>436.34</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>152.37</td>
<td>152.37</td>
</tr>
<tr>
<td>Phenol</td>
<td>145.36</td>
<td>145.36</td>
</tr>
<tr>
<td>Propylene</td>
<td>604.77</td>
<td>604.77</td>
</tr>
<tr>
<td>Styrene</td>
<td>133.41</td>
<td>133.41</td>
</tr>
<tr>
<td>Toluene</td>
<td>935.95</td>
<td>935.95</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>185.50</td>
<td>185.50</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>185.57</td>
<td>185.57</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>58.66</td>
<td>58.66</td>
</tr>
<tr>
<td>Water</td>
<td>9,044.47</td>
<td>9,044.47</td>
</tr>
</tbody>
</table>

**Design Data:**  
**Type:** Centrifugal Compressor  
**Material:** Cast Iron/Carbon-Steel  
**Power Requirement:** 7,232 hp

**Utilities:**  
Electricity at 5,393 kW

**Cost Information:**  
**Purchase Cost per unit:** $2,395,294.44  
**Total Bare Module Cost:** $6,247,406.96
<table>
<thead>
<tr>
<th><strong>Pump</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification:</strong></td>
</tr>
<tr>
<td>Item No.</td>
</tr>
<tr>
<td>No. Required</td>
</tr>
<tr>
<td><strong>Function:</strong></td>
</tr>
<tr>
<td><strong>Operation:</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Performance of Unit</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inlet</strong></td>
</tr>
<tr>
<td>Stream I.D.</td>
</tr>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Phase</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
</tr>
<tr>
<td>Water</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Design Data:</strong></th>
<th><strong>Type:</strong></th>
<th>Centrifugal Pump</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Material:</strong></td>
<td>Cast Iron</td>
<td></td>
</tr>
<tr>
<td><strong>Flow Rate:</strong></td>
<td>247 gpm</td>
<td></td>
</tr>
<tr>
<td><strong>Head:</strong></td>
<td>106 ft</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th><strong>Utilities:</strong></th>
<th>Electricity at 6 kW</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th><strong>Cost Information:</strong></th>
<th><strong>Purchase Cost per unit:</strong></th>
<th>$4,466.16</th>
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</thead>
<tbody>
<tr>
<td><strong>Total Bare Module Cost:</strong></td>
<td>$16,713.27</td>
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</table>
## Condenser

<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item Fixed Head Shell and Tube Heat Exchanger</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>Cn-301</td>
</tr>
<tr>
<td>No. Required</td>
<td>4</td>
</tr>
</tbody>
</table>

**Function:**
To cool vapor product in preparation for extraction of valuable products

**Operation:**
Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet</th>
<th>Outlet</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>S308</td>
<td>S306</td>
<td>S305</td>
<td>S309</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>0</td>
<td>145</td>
<td>326</td>
<td>5</td>
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<tr>
<td>Phase</td>
<td>Liquid</td>
<td>Vapor/Liquid</td>
<td>Vapor</td>
<td>Vapor/Liquid</td>
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<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>55,000.00</td>
<td>55,000.00</td>
<td>52,001.10</td>
<td>52,001.10</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Mass Flow Rate (kg/hr)</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>744.96</td>
<td>744.96</td>
</tr>
<tr>
<td>Benzoquinone</td>
<td>54.76</td>
<td>54.76</td>
</tr>
<tr>
<td>Butadiene</td>
<td>166.85</td>
<td>166.85</td>
</tr>
<tr>
<td>Butene</td>
<td>66.38</td>
<td>66.38</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>23,626.40</td>
<td>23,626.40</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>11,393.60</td>
<td>11,393.60</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>37.09</td>
<td>37.09</td>
</tr>
<tr>
<td>Ethylene</td>
<td>1,508.74</td>
<td>1,508.74</td>
</tr>
<tr>
<td>Indene</td>
<td>212.30</td>
<td>212.30</td>
</tr>
<tr>
<td>Methane</td>
<td>2,314.63</td>
<td>2,314.63</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>436.33</td>
<td>436.33</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>152.37</td>
<td>152.37</td>
</tr>
<tr>
<td>Phenol</td>
<td>145.35</td>
<td>145.35</td>
</tr>
<tr>
<td>Propylene</td>
<td>602.97</td>
<td>602.97</td>
</tr>
<tr>
<td>Styrene</td>
<td>133.29</td>
<td>133.29</td>
</tr>
<tr>
<td>Toluene</td>
<td>932.41</td>
<td>932.41</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>185.38</td>
<td>185.38</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>185.38</td>
<td>185.38</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>58.62</td>
<td>58.62</td>
</tr>
<tr>
<td>Water</td>
<td>55,000.00</td>
<td>55,000.00</td>
</tr>
</tbody>
</table>

### Design Data:
- **Type:** Shell & Tube, Fixed Head
- **Flow Type:** Counter-Current
- **Material:** Carbon Steel
- **Dimensions:** Surface Area = 17,969 ft²
- **Heat Duty:** 44 MMBtu/hr

### Utilities:
- Cooling water at ambient temperature, 55,000 kg/hr

### Cost Information:
- Purchase Cost per unit: $63,829.61
- Bare Module Cost per unit: $255,318.45
- Total Bare Module Cost: $990,196.45
### Identification:
- **Item**: Three Phase Flash Drum
- **Item No.**: Fl-301
- **No. Required**: 1

### Function:
To separate volatile, organic, and aqueous phases in product stream

### Operation:
Continuous

#### Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet</th>
<th>Outlet 1</th>
<th>Outlet 2</th>
<th>Outlet 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>744.96</td>
<td>141.40</td>
<td>trace</td>
<td>603.57</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>54.76</td>
<td>0.15</td>
<td>trace</td>
<td>54.61</td>
</tr>
<tr>
<td>Butadiene</td>
<td>166.85</td>
<td>145.87</td>
<td>trace</td>
<td>20.98</td>
</tr>
<tr>
<td>Butene</td>
<td>66.38</td>
<td>59.28</td>
<td>trace</td>
<td>7.10</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>23,626.40</td>
<td>23,620.50</td>
<td>trace</td>
<td>5.88</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>11,393.60</td>
<td>11,315.70</td>
<td>2.67</td>
<td>75.19</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>37.09</td>
<td>0.64</td>
<td>trace</td>
<td>36.45</td>
</tr>
<tr>
<td>Ethylene</td>
<td>1,508.74</td>
<td>1,501.27</td>
<td>trace</td>
<td>7.46</td>
</tr>
<tr>
<td>Indene</td>
<td>212.30</td>
<td>0.33</td>
<td>trace</td>
<td>211.97</td>
</tr>
<tr>
<td>Methane</td>
<td>2,314.63</td>
<td>2,312.70</td>
<td>trace</td>
<td>1.93</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>436.33</td>
<td>0.16</td>
<td>trace</td>
<td>436.17</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>152.37</td>
<td>152.34</td>
<td>trace</td>
<td>0.03</td>
</tr>
<tr>
<td>Phenol</td>
<td>145.35</td>
<td>0.19</td>
<td>1.12</td>
<td>144.03</td>
</tr>
<tr>
<td>Propylene</td>
<td>602.97</td>
<td>584.89</td>
<td>trace</td>
<td>18.08</td>
</tr>
<tr>
<td>Styrene</td>
<td>133.29</td>
<td>1.89</td>
<td>trace</td>
<td>131.40</td>
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<tr>
<td>Toluene</td>
<td>932.41</td>
<td>52.52</td>
<td>trace</td>
<td>879.90</td>
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<tr>
<td>m-Xylene</td>
<td>185.38</td>
<td>2.75</td>
<td>trace</td>
<td>182.57</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>185.38</td>
<td>2.93</td>
<td>trace</td>
<td>182.45</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>58.62</td>
<td>0.68</td>
<td>trace</td>
<td>57.94</td>
</tr>
<tr>
<td>Water</td>
<td>9,043.33</td>
<td>15.93</td>
<td>9,009.31</td>
<td>18.13</td>
</tr>
</tbody>
</table>

#### Design Data:
- **Type**: Vertical Vessel
- **Material**: Carbon Steel
- **Dimensions**:
  - Diameter: 3.07 m
  - Height: 9.22 m
- **Heat Duty**: 1.15 MMBtu/hr

#### Utilities:
- **Purchase Cost**: $19,962.95
- **Total Bare Module Cost**: $83,045.87
## Identification
- **Item**: Centrifugal Blower
- **Item No.**: B-301
- **No. Required**: 1

## Function
To transport the volatile components of the product stream to the heat integration section

## Operation
- **Continuous**

## Performance of Unit
<table>
<thead>
<tr>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td></td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>5</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>9</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>39,912.10</td>
</tr>
<tr>
<td>Benzene</td>
<td>141.39</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>0.15</td>
</tr>
<tr>
<td>Butadiene</td>
<td>145.87</td>
</tr>
<tr>
<td>Butene</td>
<td>59.28</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>23,620.50</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>11,315.70</td>
</tr>
<tr>
<td>Ethybenzene</td>
<td>0.64</td>
</tr>
<tr>
<td>Ethylene</td>
<td>1,501.27</td>
</tr>
<tr>
<td>Indene</td>
<td>0.33</td>
</tr>
<tr>
<td>Methane</td>
<td>2,312.70</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0.16</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>152.34</td>
</tr>
<tr>
<td>Phenol</td>
<td>0.19</td>
</tr>
<tr>
<td>Propylene</td>
<td>584.89</td>
</tr>
<tr>
<td>Styrene</td>
<td>1.89</td>
</tr>
<tr>
<td>Toluene</td>
<td>52.52</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>2.75</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>2.93</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>0.68</td>
</tr>
<tr>
<td>Water</td>
<td>15.93</td>
</tr>
</tbody>
</table>

## Design Data
- **Type**: Centrifugal Blower
- **Material**: Cast Iron/Carbon-Steel
- **Specific Heat Ratio**: 1.4
- **Volumetric Capacity**: 1,974 ft³/min

## Utilities
- **Electricity at 36 kW**

## Cost Information
- **Purchase Cost per unit**: $222,084.57
- **Total Bare Module Cost**: $251,843.90
## Identification
Item: Centrifugal Compressor & Electric Motor

Item No.: P-302
No. Required: 1

## Function
To transport aqueous phase of vapor stream to waste water treatment facility

## Operation
Continuous

## Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet S312</th>
<th>Outlet S318</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>9</td>
<td>10.7</td>
</tr>
<tr>
<td>Phase</td>
<td>Liquid</td>
<td>Liquid</td>
</tr>
</tbody>
</table>

| Mass Flow Rate (kg/hr) | 9,013.11 | 9,013.11 |
| Benzene              | trace    | trace     |
| Benzofuran           | trace    | trace     |
| Butadiene            | trace    | trace     |
| Butene               | trace    | trace     |
| Carbon Dioxide       | trace    | trace     |
| Carbon Monoxide      | 2.67     | 2.67      |
| Ethylbenzene         | trace    | trace     |
| Ethylene             | trace    | trace     |
| Indene               | trace    | trace     |
| Methane              | trace    | trace     |
| Naphthalene          | trace    | trace     |
| Nitrogen             | trace    | trace     |
| Phenol               | 1.12     | 1.12      |
| Propylene            | trace    | trace     |
| Styrene              | trace    | trace     |
| Toluene              | trace    | trace     |
| m-Xylene             | trace    | trace     |
| p-Xylene             | trace    | trace     |
| o-Xylene             | trace    | trace     |
| Water                | 9,009.31 | 9,009.31  |

## Design Data
Type: Centrifugal Pump
Material: Cast Iron
Flow Rate: 40.64 gpm
Head: 59 ft

## Utilities
Electricity at .5 kW

## Cost Information
Purchase Cost per unit: $3,273.40
Total Bare Module Cost: $12,249.69
### Distillation Column

<table>
<thead>
<tr>
<th>Identification: Item</th>
<th>Item No.</th>
<th>Di-301</th>
<th>No. Required</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function:</strong></td>
<td>To separate the valuable aromatic products from the high-boiling fractions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Operation:</strong></td>
<td>Continuous</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Feed</th>
<th>Overhead</th>
<th>Side-Draw</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream I.D.</strong></td>
<td>S313</td>
<td>S316</td>
<td>S315</td>
<td>S317</td>
</tr>
<tr>
<td><strong>Temperature (°C)</strong></td>
<td>5</td>
<td>30</td>
<td>30</td>
<td>314</td>
</tr>
<tr>
<td><strong>Pressure (bar)</strong></td>
<td>9</td>
<td>4.76</td>
<td>4.76</td>
<td>8.5</td>
</tr>
<tr>
<td><strong>Phase</strong></td>
<td>Vapor/Liquid</td>
<td>Vapor/Liquid</td>
<td>Vapor</td>
<td>Liquid</td>
</tr>
<tr>
<td><strong>Mass Flow Rate (kg/hr)</strong></td>
<td>3,024.22</td>
<td>2,309.30</td>
<td>24.58</td>
<td>690.35</td>
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<tr>
<td>Benzene</td>
<td>586.91</td>
<td>586.32</td>
<td>0.59</td>
<td>trace</td>
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<tr>
<td>Benzo[</td>
<td>54.59</td>
<td>38.12</td>
<td>trace</td>
<td>16.47</td>
</tr>
<tr>
<td>Butadiene</td>
<td>17.58</td>
<td>17.23</td>
<td>0.34</td>
<td>trace</td>
</tr>
<tr>
<td>Butene</td>
<td>5.91</td>
<td>5.77</td>
<td>0.13</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>4.59</td>
<td>0.69</td>
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<td>-</td>
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<td>Carbon Monoxide</td>
<td>59.86</td>
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<td>-</td>
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<td>36.37</td>
<td>trace</td>
<td>trace</td>
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<tr>
<td>Ethylene</td>
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<td>1.69</td>
<td>-</td>
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<td>0.51</td>
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<td>Naphthalene</td>
<td>436.15</td>
<td>trace</td>
<td>trace</td>
<td>436.15</td>
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<td>Nitrogen</td>
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<td>0.02</td>
<td>-</td>
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<td>Phenol</td>
<td>143.99</td>
<td>110.71</td>
<td>trace</td>
<td>33.28</td>
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<tr>
<td>Propylene</td>
<td>14.63</td>
<td>13.57</td>
<td>1.06</td>
<td>trace</td>
</tr>
<tr>
<td>Styrene</td>
<td>131.16</td>
<td>131.06</td>
<td>0.01</td>
<td>0.10</td>
</tr>
<tr>
<td>Toluene</td>
<td>873.14</td>
<td>872.88</td>
<td>0.26</td>
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</tr>
<tr>
<td>m-Xylene</td>
<td>182.09</td>
<td>182.21</td>
<td>0.02</td>
<td>trace</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>182.09</td>
<td>182.07</td>
<td>0.02</td>
<td>trace</td>
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<tr>
<td>o-Xylene</td>
<td>57.85</td>
<td>57.84</td>
<td>trace</td>
<td>trace</td>
</tr>
<tr>
<td>Water</td>
<td>17.78</td>
<td>17.71</td>
<td>0.07</td>
<td>trace</td>
</tr>
</tbody>
</table>

#### Design Data:

- **Type:** Tower
- **Material:** Carbon Steel
- **Tray Type:** Sieve
- **Dimensions:** Diameter 3.16 ft, Height 53 ft
- **Number of Stages:** 27
- **Reflux Ratio:** 0.714
- **Distillate/Feed Ratio:** 0.771
- **Condenser Heat Duty:** 2.37 MMBtu/hr
- **Reboiler Heat Duty:** 2.86 MMBtu/hr

#### Utilities:

- **Electricity at 1535 kWh**

#### Cost Information:

- **Purchase Cost per unit:** $86,407.71
- **Total Bare Module Cost:** $359,456.07
### Distillation Column

<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item No.</th>
<th>Di-302</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. Required</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Function:** To separate BTX and other valuable aromatic from phenol

**Operation:** Continuous

#### Performance of Unit

<table>
<thead>
<tr>
<th>Stream ID.</th>
<th>Feed</th>
<th>Overhead</th>
<th>Bottoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>S316</td>
<td></td>
<td>S318</td>
<td>S319</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>30</td>
<td>15</td>
<td>237</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor/Liquid</td>
<td>Liquid</td>
<td>Liquid</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>2,309.30</td>
<td>2,193.84</td>
<td>115.47</td>
</tr>
<tr>
<td>Benzene</td>
<td>586.32</td>
<td>586.32</td>
<td>trace</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>38.12</td>
<td>24.97</td>
<td>24.33</td>
</tr>
<tr>
<td>Butadiene</td>
<td>17.23</td>
<td>17.23</td>
<td>trace</td>
</tr>
<tr>
<td>Butene</td>
<td>5.77</td>
<td>5.78</td>
<td>trace</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0.69</td>
<td>0.69</td>
<td>trace</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>44.39</td>
<td>44.39</td>
<td>trace</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>36.37</td>
<td>36.37</td>
<td>trace</td>
</tr>
<tr>
<td>Ethylene</td>
<td>4.24</td>
<td>4.24</td>
<td>trace</td>
</tr>
<tr>
<td>Indene</td>
<td>7.60</td>
<td>0.63</td>
<td>7.35</td>
</tr>
<tr>
<td>Methane</td>
<td>0.51</td>
<td>0.51</td>
<td>trace</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>trace</td>
<td>trace</td>
<td>trace</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>trace</td>
<td>trace</td>
<td>trace</td>
</tr>
<tr>
<td>Phenol</td>
<td>110.71</td>
<td>15.36</td>
<td>83.30</td>
</tr>
<tr>
<td>Propylene</td>
<td>13.57</td>
<td>13.58</td>
<td>trace</td>
</tr>
<tr>
<td>Styrene</td>
<td>131.06</td>
<td>131.05</td>
<td>0.39</td>
</tr>
<tr>
<td>Toluene</td>
<td>872.88</td>
<td>872.88</td>
<td>trace</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>182.21</td>
<td>182.21</td>
<td>0.02</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>182.07</td>
<td>182.07</td>
<td>0.02</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>57.84</td>
<td>57.84</td>
<td>0.05</td>
</tr>
<tr>
<td>Water</td>
<td>17.71</td>
<td>17.71</td>
<td>trace</td>
</tr>
</tbody>
</table>

#### Design Data:

- **Type:** Tower
- **Material:** Carbon Steel
- **Tray Type:** Sieve
- **Dimensions:** Diameter
- **Height:**
- **Number of Stages:** 15
- **Reflux Ratio:** 0.75
- **Distillate/Feed Ratio:** 0.95
- **Condenser Heat Duty:** 2.28 MMBtu/hr
- **Reboiler Heat Duty:** 2.27 MMBtu/hr

**Utilities:** Electricity at 1335 kWh

**Cost Information:**
- **Purchase Cost per unit:** $67,586.17
- **Total Bare Module Cost:** $281,158.45
## 8. 4 Section 400: Heat Integration

<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item</th>
<th>Centrifugal Blower</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>B-401</td>
<td></td>
</tr>
<tr>
<td>No. Required</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

**Function:** To transport volatile stream from solid/vapor cyclone to the heat integration network

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th><strong>Inlet</strong></th>
<th><strong>Outlet</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S211</td>
<td>S401</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>700</td>
<td>907</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1</td>
<td>2.03</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>398,486.00</td>
<td>398,486.00</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>27,944.60</td>
<td>27,944.60</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>299,821.00</td>
<td>299,821.00</td>
</tr>
<tr>
<td>Oxygen</td>
<td>70,719.60</td>
<td>70,719.60</td>
</tr>
</tbody>
</table>

**Design Data:**
- Type: Centrifugal Compressor
- Material: Cast Iron/Carbon-Steel
- Power Requirement: 40,000 hp

**Utilities:** Electricity at 256 kW

**Cost Information:**
- Purchase Cost per unit: $9,234,285.72
- Bare Module Cost per unit: $10,471,680.00
- Total Bare Module Cost: $20,943,360.00
# Heat Exchanger

**Identification:** Fixed Head Shell and Tube Heat Exchanger  
**Item No.:** HX-401  
**No. Required:** 1

**Function:** To cool down recycle volatile stream to be used as carrier gas in the circulating fluidized bed

**Operation:** Continuous

## Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th></th>
<th>Tube Side</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream I.D.</strong></td>
<td></td>
<td>S311</td>
<td>S402</td>
<td>S401</td>
</tr>
<tr>
<td><strong>Temperature (°C)</strong></td>
<td></td>
<td>28</td>
<td>600</td>
<td>1000</td>
</tr>
<tr>
<td><strong>Pressure (bar)</strong></td>
<td></td>
<td>10.03</td>
<td>10.03</td>
<td>2.72</td>
</tr>
<tr>
<td><strong>Phase</strong></td>
<td></td>
<td>Vapor</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td><strong>Mass Flow Rate (kg/hr)</strong></td>
<td>39,912.10</td>
<td>39,912.10</td>
<td>398,486.00</td>
<td>398,486.00</td>
</tr>
<tr>
<td><strong>Benzene</strong></td>
<td>141.39</td>
<td>141.39</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Benzofuran</strong></td>
<td>0.15</td>
<td>0.15</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Butadiene</strong></td>
<td>145.87</td>
<td>145.87</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Butene</strong></td>
<td>59.28</td>
<td>59.28</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Carbon Dioxide</strong></td>
<td>23,620.50</td>
<td>23,620.50</td>
<td>27,944.60</td>
<td>27,944.60</td>
</tr>
<tr>
<td><strong>Carbon Monoxide</strong></td>
<td>11,315.70</td>
<td>11,315.70</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Ethylbenzene</strong></td>
<td>0.64</td>
<td>0.64</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Ethylene</strong></td>
<td>1,501.27</td>
<td>1,501.27</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Indene</strong></td>
<td>0.33</td>
<td>0.33</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Methane</strong></td>
<td>2,312.70</td>
<td>2,312.70</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Naphthalene</strong></td>
<td>0.16</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Nitrogen</strong></td>
<td>152.34</td>
<td>152.34</td>
<td>299,821.00</td>
<td>299,821.00</td>
</tr>
<tr>
<td><strong>Oxygen</strong></td>
<td>-</td>
<td>-</td>
<td>70,719.60</td>
<td>70,719.60</td>
</tr>
<tr>
<td><strong>Phenol</strong></td>
<td>0.19</td>
<td>0.19</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Propylene</strong></td>
<td>584.89</td>
<td>584.89</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Styrene</strong></td>
<td>1.89</td>
<td>1.89</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Toluene</strong></td>
<td>52.52</td>
<td>52.52</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>m-Xylene</strong></td>
<td>2.75</td>
<td>2.75</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>p-Xylene</strong></td>
<td>2.93</td>
<td>2.93</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>o-Xylene</strong></td>
<td>0.68</td>
<td>0.68</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Water</strong></td>
<td>15.93</td>
<td>15.93</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

## Design Data:

**Type:** Shell & Tube, Fixed Head  
**Flow Type:** Counter-Current  
**Material:** Carbon Steel  
**Tube Length:** 20 ft  
**Dimensions:** Surface Area: 167 ft²  
**Heat Duty:** 28 MMBtu/hr

## Utilities:

Volatile stream from catalyst regenerator at 39,912.1 kg/hr

## Cost Information:

**Purchase Cost:** $9,422.20  
**Total Bare Module Cost:** $34,139.58
<table>
<thead>
<tr>
<th>Compressor</th>
<th>Identification:</th>
<th>Item Centrifugal Compressor</th>
<th>Item No. C-401</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. Required</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Function:</td>
<td>To transport nitrogen carrier gas for preheating before entering the circulating fluidized bed riser</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Operation:</td>
<td>Continuous</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Performance of Unit</th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S404</td>
<td>S405</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
<td>179</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.01</td>
<td>3.77</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>100.00</td>
<td>100.00</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>100.00</td>
<td>100.00</td>
</tr>
</tbody>
</table>

| Design Data: | Type: Centrifugal Compressor |
| Material: Cast Iron/Carbon-Steel |
| Power Requirement: 6.64 hp |

| Utilities: | Electricity at 5 kW |

| Cost Information: | Purchase Cost: $13,292.84 |
| Total Bare Module Cost: $34,670.39 |
### Heat Exchanger

**Identification:** Fixed Head Shell and Tube Heat Exchanger

<table>
<thead>
<tr>
<th>Item No.</th>
<th>HX-402</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. Required</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function:** To heat up carrier gas stream to circulating fluidized catalytic reactor

**Operation:** Continuous

<table>
<thead>
<tr>
<th>Performance of Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Shell Side</strong></td>
</tr>
<tr>
<td><strong>Inlet</strong></td>
</tr>
<tr>
<td>Stream I.D.</td>
</tr>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Phase</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
</tr>
</tbody>
</table>

| | **Shell Side** | **Tube Side** |
| Benzene | - | - | 92.79 | 92.79 |
| Benzo furan | - | - | 0.10 | 0.10 |
| Butadiene | - | - | 95.73 | 95.73 |
| Butene | - | - | 38.90 | 38.90 |
| Carbon Dioxide | - | - | 15,501.00 | 15,501.00 |
| Carbon Monoxide | - | - | 7,425.98 | 7,425.98 |
| Ethybenzene | - | - | 0.42 | 0.42 |
| Ethylene | - | - | 985.21 | 985.21 |
| Indene | - | - | 0.22 | 0.22 |
| Methane | - | - | 1,517.71 | 1,517.71 |
| Naphthalene | - | - | 0.10 | 0.10 |
| Nitrogen | 100.00 | 100.00 | 99.97 | 99.97 |
| Phenol | - | - | 0.13 | 0.13 |
| Propylene | - | - | 383.83 | 383.83 |
| Styrene | - | - | 1.24 | 1.24 |
| Toluene | - | - | 34.47 | 34.47 |
| m-Xylene | - | - | 1.81 | 1.81 |
| p-Xylene | - | - | 1.92 | 1.92 |
| o-Xylene | - | - | 0.45 | 0.45 |
| Water | - | - | 10.45 | 10.45 |

**Design Data:**
- Type: Shell & Tube, Fixed Head
- Flow Type: Counter-Current
- Material: Carbon Steel
- Dimensions: Surface Area: 1.44 ft²
- Heat Duty: 42.5 MBtu/hr

**Utilities:**
- Hot recycle stream, 26,192.4 kg/hr

**Cost Information:**
- Purchase Cost: $15,778.35
- Total Bare Module Cost: $61,192.86
<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item Centrifugal Compressor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>C-402</td>
</tr>
<tr>
<td>No. Required</td>
<td>1</td>
</tr>
<tr>
<td>Function:</td>
<td>To transport carrier gas purge stream to heat up air to be used for drying the biomass</td>
</tr>
<tr>
<td>Operation:</td>
<td>Continuous</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Performance of Unit</strong></th>
<th><strong>Inlet</strong></th>
<th><strong>Outlet</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S407</td>
<td>S408</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>599</td>
<td>623</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>12.44</td>
<td>14.17</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>26,192.40</td>
<td>26,192.40</td>
</tr>
<tr>
<td>Benzene</td>
<td>92.79</td>
<td>92.79</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>Butadiene</td>
<td>95.73</td>
<td>95.73</td>
</tr>
<tr>
<td>Butene</td>
<td>38.90</td>
<td>38.90</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>15,501.00</td>
<td>15,501.00</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>7,425.98</td>
<td>7,425.98</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0.42</td>
<td>0.42</td>
</tr>
<tr>
<td>Ethylene</td>
<td>985.21</td>
<td>985.21</td>
</tr>
<tr>
<td>Indene</td>
<td>0.22</td>
<td>0.22</td>
</tr>
<tr>
<td>Methane</td>
<td>1,517.71</td>
<td>1,517.71</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>99.97</td>
<td>99.97</td>
</tr>
<tr>
<td>Phenol</td>
<td>0.13</td>
<td>0.13</td>
</tr>
<tr>
<td>Propylene</td>
<td>383.83</td>
<td>383.83</td>
</tr>
<tr>
<td>Styrene</td>
<td>1.24</td>
<td>1.24</td>
</tr>
<tr>
<td>Toluene</td>
<td>34.47</td>
<td>34.47</td>
</tr>
<tr>
<td>m-Xylene</td>
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<td>1.81</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>1.92</td>
<td>1.92</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>0.45</td>
<td>0.45</td>
</tr>
<tr>
<td>Water</td>
<td>10.45</td>
<td>10.45</td>
</tr>
</tbody>
</table>

**Design Data:**
- **Type:** Centrifugal Compressor
- **Material:** Cast Iron/Carbon-Steel
- **Power Requirement:** 392 hp

**Utilities:**
- Electricity at 292 kW

**Cost Information:**
- **Purchase Cost:** $232,584.64
- **Total Bare Module Cost:** $606,627.25
<table>
<thead>
<tr>
<th>Identification:</th>
<th><strong>Item</strong></th>
<th>Centrifugal Blower</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>B-402</td>
<td></td>
</tr>
<tr>
<td>No. Required</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Function:** To transport air to be used for drying the biomass

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S409</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.01</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>30,000.00</td>
</tr>
<tr>
<td>Air</td>
<td>30,000.00</td>
</tr>
</tbody>
</table>

**Design Data:**
- **Type:** Centrifugal Blower
- **Material:** Cast Iron/Carbon-Steel
- **Specific Heat Ratio:** 1.4
- **Volumetric Capacity:** 14,917 ft³/min

**Utilities:**
- Electricity at 272 kW

**Cost Information:**
- **Purchase Cost:** $132,398.03
- **Total Bare Module Cost:** $150,139.37
## Heat Exchanger

**Identification:** Item Fixed Head Shell and Tube Heat Exchanger  
Item No. HX-403  
No. Required 1

**Function:** To transfer heat to air stream from the carrier gas purge stream to allow biomass to be dried

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inlet</strong></td>
<td><strong>Outlet</strong></td>
<td><strong>Inlet</strong></td>
</tr>
<tr>
<td>Stream I.D.</td>
<td>S410</td>
<td>S116</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>136</td>
<td>300</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>2.74</td>
<td>2.74</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>30,000.00</td>
<td>30,000.00</td>
</tr>
<tr>
<td>Air</td>
<td>30,000.00</td>
<td>30,000.00</td>
</tr>
<tr>
<td>Benzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butadiene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Indene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Methane</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Phenol</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Propylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Styrene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Toluene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

### Design Data:
- **Type:** Shell & Tube, Fixed Head  
- **Flow Type:** Counter-Current  
- **Material:** Carbon Steel  
- **Dimensions:** Surface Area: 52.31 ft²  
- **Heat Duty:** 5 MBtu/hr

### Utilities:
- Hot recycle stream, 26,192.4 kg/hr

### Cost Information:
- **Purchase Cost:** $9,767.90  
- **Total Bare Module Cost:** $33,406.00
<table>
<thead>
<tr>
<th>Identification:</th>
<th>Item</th>
<th>Centrifugal Compressor &amp; Electric Motor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td></td>
<td>C-401</td>
</tr>
<tr>
<td>No. Required</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Function:** To transport cooling water to low pressure steam economizers in heat integration section.

**Operation:** Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th>Inlet</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S412</td>
<td>S413</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
<td>26</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1.01</td>
<td>179</td>
</tr>
<tr>
<td>Phase</td>
<td>Liquid</td>
<td>Liquid</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>166,537.00</td>
<td>166,537.00</td>
</tr>
<tr>
<td>Water</td>
<td>166,537.00</td>
<td>166,537.00</td>
</tr>
</tbody>
</table>

**Design Data:**
- **Type:** Centrifugal Compressor
- **Material:** Cast Iron/Carbon-Steel
- **Power Requirement:** 1,452 hp

**Utilities:** Electricity at 1,083 kW

**Cost Information:**
- **Purchase Cost per unit:** $4,954.06
- **Total Bare Module Cost:** $18,539.04
# Heat Exchanger

**Identification:** Item Fixed Head Shell and Tube Heat Exchanger  
**Item No.** HX-404  
**No. Required** 1

**Function:** To cool down flue gases produced from catalytic regeneration and co-produce low pressure steam

**Operation:** Continuous

<table>
<thead>
<tr>
<th><strong>Performance of Unit</strong></th>
<th><strong>Shell Side</strong></th>
<th><strong>Tube Side</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream I.D.</strong></td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td></td>
<td>S415</td>
<td>S424</td>
</tr>
<tr>
<td><strong>Temperature (°C)</strong></td>
<td>26</td>
<td>480</td>
</tr>
<tr>
<td><strong>Pressure (bar)</strong></td>
<td>179</td>
<td>179</td>
</tr>
<tr>
<td><strong>Phase</strong></td>
<td>Liquid</td>
<td>Vapor</td>
</tr>
<tr>
<td><strong>Mass Flow Rate (kg/hr)</strong></td>
<td>3,200.00</td>
<td>3,200.00</td>
</tr>
<tr>
<td>Benzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butadiene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Butene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Ethylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Indene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Methane</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Phenol</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Propylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Styrene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Toluene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>3,200.00</td>
<td>3,200.00</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

**Design Data:**
- **Type:** Shell & Tube, Fixed Head  
- **Flow Type:** Counter-Current  
- **Material:** Carbon Steel  
- **Dimensions:** Surface Area: 642 ft²  
- **Heat Duty:** 10 MBtu/hr

**Utilities:**

**Cost Information:**  
- **Purchase Cost:** $12,686.45  
- **Total Bare Module Cost:** $70,394.71
### Heat Exchanger

**Identification:**
- Item: Fixed Head Shell and Tube Heat Exchanger
- Item No.: HX-405
- No. Required: 1

**Function:**
To cool down flue gases from the catalytic regenerator and co-generate low pressure steam

**Operation:**
Continuous

<table>
<thead>
<tr>
<th>Performance of Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Shell Side</strong></td>
</tr>
<tr>
<td>Stream I.D.</td>
</tr>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Phase</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
</tr>
<tr>
<td>Carbon Moxonide</td>
</tr>
<tr>
<td>Nitrogen</td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
<tr>
<td>Water</td>
</tr>
</tbody>
</table>

**Design Data:**
- Type: Shell & Tube, Fixed Head
- Flow Type: Counter-Current
- Material: Carbon Steel
- Dimensions: Surface Area: 288 ft²
- Heat Duty: 82.692 MBtu/hr

**Utilities:**

**Cost Information:**
- Purchase Cost: $10,193.01
- Total Bare Module Cost: $55,060.23
<table>
<thead>
<tr>
<th>Identification: Item Combustor</th>
<th>Item No. R-401</th>
<th>No. Required 1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function:</strong></td>
<td>To combust purged volatile streams for their heating value</td>
<td></td>
</tr>
<tr>
<td><strong>Operation:</strong></td>
<td>Continuous</td>
<td></td>
</tr>
</tbody>
</table>

**Performance of Unit**

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Inlet 3</th>
<th>Inlet 4</th>
<th>Outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>759</td>
<td>193</td>
<td>237</td>
<td>30</td>
<td>314</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>2.03</td>
<td>14.17</td>
<td>4</td>
<td>4.76</td>
<td>8.5</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>398,486.00</td>
<td>26,192.40</td>
<td>115,465</td>
<td>24.58</td>
<td>690.35</td>
</tr>
<tr>
<td>Benzene</td>
<td>-</td>
<td>92.79</td>
<td>trace</td>
<td>0.59</td>
<td>trace</td>
</tr>
<tr>
<td>Benzofuran</td>
<td>-</td>
<td>0.10</td>
<td>24.33</td>
<td>trace</td>
<td>16.47</td>
</tr>
<tr>
<td>Butadiene</td>
<td>-</td>
<td>95.73</td>
<td>trace</td>
<td>0.34</td>
<td>trace</td>
</tr>
<tr>
<td>Butene</td>
<td>-</td>
<td>38.90</td>
<td>trace</td>
<td>0.13</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>27,944.60</td>
<td>15,501.00</td>
<td>trace</td>
<td>3.90</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>-</td>
<td>7,425.98</td>
<td>trace</td>
<td>15.47</td>
<td>-</td>
</tr>
<tr>
<td>Ethylene</td>
<td>-</td>
<td>0.42</td>
<td>trace</td>
<td>trace</td>
<td>trace</td>
</tr>
<tr>
<td>Indene</td>
<td>-</td>
<td>985.21</td>
<td>trace</td>
<td>1.69</td>
<td>-</td>
</tr>
<tr>
<td>Methane</td>
<td>-</td>
<td>0.22</td>
<td>7.35</td>
<td>trace</td>
<td>204.33</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>-</td>
<td>1,517.71</td>
<td>trace</td>
<td>1.00</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>299,821.00</td>
<td>99.97</td>
<td>trace</td>
<td>0.02</td>
<td>-</td>
</tr>
<tr>
<td>Oxygen</td>
<td>70,719.60</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Phenol</td>
<td>-</td>
<td>0.13</td>
<td>83.30</td>
<td>trace</td>
<td>33.28</td>
</tr>
<tr>
<td>Propylene</td>
<td>-</td>
<td>383.83</td>
<td>trace</td>
<td>1.06</td>
<td>trace</td>
</tr>
<tr>
<td>Styrene</td>
<td>-</td>
<td>1.24</td>
<td>0.39</td>
<td>0.01</td>
<td>0.10</td>
</tr>
<tr>
<td>Toluene</td>
<td>-</td>
<td>34.37</td>
<td>trace</td>
<td>0.26</td>
<td>trace</td>
</tr>
<tr>
<td>Water</td>
<td>-</td>
<td>10.45</td>
<td>0.02</td>
<td>0.02</td>
<td>trace</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>-</td>
<td>1.81</td>
<td>0.02</td>
<td>0.02</td>
<td>trace</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>-</td>
<td>0.45</td>
<td>0.05</td>
<td>trace</td>
<td>trace</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>-</td>
<td>1.92</td>
<td>trace</td>
<td>0.07</td>
<td>trace</td>
</tr>
</tbody>
</table>

**Design Data:**

- **Type:** Vertical Vessel
- **Material:** Stainless Steel with Ceramic Lined Exterior
- **Dimensions:**
  - Diameter: 12.5 ft
  - Height: 37.6 ft
- **Heat Duty:** 478 MMBtu/hr

**Utilities:**

**Cost Information:**

- **Purchase Cost:** $145,000.34
- **Total Bare Module Cost:** $603,201.41
**Heat Exchanger**

**Identification:**  
Item: Fixed Head Shell and Tube Heat Exchanger  
Item No.: HX-406  
No. Required: 1

**Function:**  
To cool down flue gases from the waste heat boiler and co-generate low pressure steam

**Operation:**  
Continuous

### Performance of Unit

<table>
<thead>
<tr>
<th>Stream I.D.</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inlet</td>
<td>Outlet</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>25</td>
<td>200</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>2.72</td>
<td>2.72</td>
</tr>
<tr>
<td>Phase</td>
<td>Liquid</td>
<td>Vapor</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>140,000.00</td>
<td>140,000.00</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Carbon Moxonide</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Oxygen</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Water</td>
<td>140,000.00</td>
<td>140,000.00</td>
</tr>
</tbody>
</table>

### Design Data:

| Type: | Shell & Tube, Fixed Head |
| Flow Type: | Counter-Current |
| Material: | Carbon Steel |
| Dimensions: | Surface Area: 7,335 ft² |
| Heat Duty | 450 MBtu/hr |

### Utilities:

### Cost Information:

- Purchase Cost: $53,692.13
- Total Bare Module Cost: $297,927.52
# 8.5 Section 500: Electricity Generation

<table>
<thead>
<tr>
<th><strong>Identification:</strong></th>
<th><strong>Item</strong></th>
<th>Steam Turbine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>T-501</td>
<td></td>
</tr>
<tr>
<td>No. Required</td>
<td>8</td>
<td></td>
</tr>
</tbody>
</table>

**Function:** To generate electricity from high pressure steam generated as a byproduct of the heat integration network

**Operation:** Continuous

## Performance of Unit

<table>
<thead>
<tr>
<th></th>
<th><em>Inlet</em></th>
<th><em>Outlet</em></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream I.D.</td>
<td>S501</td>
<td>S502</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>540</td>
<td>83</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>179</td>
<td>0.5</td>
</tr>
<tr>
<td>Phase</td>
<td>Vapor</td>
<td>Vapor/Liquid</td>
</tr>
<tr>
<td>Mass Flow Rate (kg/hr)</td>
<td>166,537.00</td>
<td>166,537.00</td>
</tr>
<tr>
<td>Water</td>
<td>166,537.00</td>
<td>166,537.00</td>
</tr>
</tbody>
</table>

**Design Data:**

<table>
<thead>
<tr>
<th></th>
<th>Type:</th>
<th>Power-Recorvery Turbine</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Subtype:</td>
<td>Gas Expander with Vacuum</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Discharge</td>
</tr>
<tr>
<td>Power Extracted:</td>
<td>8000 hp</td>
<td></td>
</tr>
</tbody>
</table>

**Utilities:** High pressure steam at 540°C, 179 bar, 166,537 kg/hr

**Cost Information:**

- Purchase Cost: $13,808,288.04
- Total Bare Module Cost: $15,658,598.64
9. FIXED CAPITAL INVESTMENT SUMMARY
9.1 Fixed Capital Investment Summary

The fixed costs of this plant derive predominantly from the equipment costs, which are shown below in Table 9.1. Cost estimates for the equipment were obtained using the parameters presented in Seider et al. [30].

Table 9.1: Summary of equipment costs

<table>
<thead>
<tr>
<th>Equipment Type</th>
<th>Purchase Cost ($)</th>
<th>Bare Module Cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Blowers &amp; Compressors</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B-201</td>
<td>515,000</td>
<td>584,000</td>
</tr>
<tr>
<td>B-202</td>
<td>1,010,000</td>
<td>1,140,000</td>
</tr>
<tr>
<td>B-203</td>
<td>2,570,000</td>
<td>2,920,000</td>
</tr>
<tr>
<td>B-301</td>
<td>222,000</td>
<td>252,000</td>
</tr>
<tr>
<td>C-301</td>
<td>2,390,000</td>
<td>6,250,000</td>
</tr>
<tr>
<td>B-401</td>
<td>18,500,000</td>
<td>20,900,000</td>
</tr>
<tr>
<td>B-402</td>
<td>132,000</td>
<td>150,000</td>
</tr>
<tr>
<td>C-401</td>
<td>13,300</td>
<td>34,700</td>
</tr>
<tr>
<td>C-402</td>
<td>233,000</td>
<td>607,000</td>
</tr>
<tr>
<td><strong>Cyclones</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cy-201</td>
<td>7,440</td>
<td>31,000</td>
</tr>
<tr>
<td>Cy-202</td>
<td>212,000</td>
<td>884,000</td>
</tr>
<tr>
<td><strong>Heat Exchangers</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HX-301</td>
<td>19,900</td>
<td>108,000</td>
</tr>
<tr>
<td>Cn-301</td>
<td>255,000</td>
<td>990,000</td>
</tr>
<tr>
<td>HX-401</td>
<td>9,440</td>
<td>34,000</td>
</tr>
<tr>
<td>HX-402</td>
<td>15,800</td>
<td>61,000</td>
</tr>
<tr>
<td>HX-403</td>
<td>9,770</td>
<td>33,400</td>
</tr>
<tr>
<td>HX-404</td>
<td>12,700</td>
<td>70,400</td>
</tr>
<tr>
<td>HX-405</td>
<td>10,200</td>
<td>55,000</td>
</tr>
<tr>
<td>HX-406</td>
<td>53,700</td>
<td>298,000</td>
</tr>
<tr>
<td><strong>Pumps and Motors</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-401_motor</td>
<td>910</td>
<td>3,400</td>
</tr>
<tr>
<td>P-401</td>
<td>4,000</td>
<td>15,100</td>
</tr>
<tr>
<td>P-301_motor</td>
<td>870</td>
<td>3,200</td>
</tr>
<tr>
<td>P-301</td>
<td>3,600</td>
<td>13,500</td>
</tr>
<tr>
<td>P-302_motor</td>
<td>370</td>
<td>1,400</td>
</tr>
<tr>
<td>P-302</td>
<td>2,900</td>
<td>10,800</td>
</tr>
</tbody>
</table>
The bare module cost for each piece of equipment was calculated by multiplying the purchase cost by a bare module factor, using a current CE Index of 567. The purchase cost includes allowances for installation labor, cost of installation materials, freight, taxes, insurance, construction overhead, and contractor expenses. Other factors that affect the total permanent investment are shown below in Table 9.2.
Table 9.2: Summary of Total Permanent Investment Factors

<table>
<thead>
<tr>
<th>Cost of Site Preparation:</th>
<th>5.00% of Total Bare Module Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Service Facilities:</td>
<td>5.00% of Total Bare Module Costs</td>
</tr>
<tr>
<td>Allocated Costs for Utility Plants and Related Facilities:</td>
<td>$0</td>
</tr>
<tr>
<td>Cost of Contingencies and Contractor Fees:</td>
<td>18.00% of Direct Permanent Investment</td>
</tr>
<tr>
<td>Cost of Land:</td>
<td>2.00% of Total Depreciable Capital</td>
</tr>
<tr>
<td>Cost of Royalties:</td>
<td>$0</td>
</tr>
<tr>
<td>Cost of Plant Start-Up:</td>
<td>10.00% of Total Depreciable Capital</td>
</tr>
</tbody>
</table>

The cost of site preparations is assumed to be 5% of the total bare module costs, which is a reasonable estimate considering the plant is located in the Gulf Coast, where there is an extensive, pre-existing infrastructure of roads and sewer lines. The cost of service facilities was also assumed to be 5% of the total bare module costs. Allocated costs for utility plants and related facilities were assumed to be zero, as this plant produces far more electricity than operation requires. The cost of contingencies and contractor fees is a combination of an allowance of 15% of the direct permanent investment (DPI) and a 3% allowance for contractor fees. This is a conservative estimate given that the BFCC process has not yet proven profitable on a commercial scale, with only a few companies yielding profit on the pilot plant scale. The cost of royalties is estimated as 2% of the total depreciable capital (TDC) and the cost of royalties is assumed to be zero, as one particular protected technology will not be licensed. Finally, the cost of plant startup has been estimated as 10% of the total depreciable capital, a conservative estimate for a process that has not yet proven feasible on a commercial scale.

The application of these factors in calculating the DPI, TDC, and total permanent investment is detailed below in Table 9.3. The total permanent investment of this project is estimated at $93 MM.
Table 9.3: Summary of Total Permanent Investment

<table>
<thead>
<tr>
<th>Investment Summary</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total Bare Module Costs:</strong></td>
<td></td>
</tr>
<tr>
<td>Fabricated Equipment</td>
<td>$ 47,502</td>
</tr>
<tr>
<td>Process Machinery</td>
<td>$ 58,283,237</td>
</tr>
<tr>
<td>Spares</td>
<td>$ -</td>
</tr>
<tr>
<td>Storage</td>
<td>$ 5,483,441</td>
</tr>
<tr>
<td>Other Equipment</td>
<td>$ 169,745</td>
</tr>
<tr>
<td>Catalysts</td>
<td>$ -</td>
</tr>
<tr>
<td>Computers, Software, Etc.</td>
<td>$ -</td>
</tr>
<tr>
<td><strong>Total Bare Module Costs:</strong></td>
<td><strong>$ 63,983,925</strong></td>
</tr>
<tr>
<td><strong>Direct Permanent Investment</strong></td>
<td></td>
</tr>
<tr>
<td>Cost of Site Preparations</td>
<td>$ 3,199,196</td>
</tr>
<tr>
<td>Cost of Service Facilities</td>
<td>$ 3,199,196</td>
</tr>
<tr>
<td>Allocated Costs for utility plants and related facilities</td>
<td>$ -</td>
</tr>
<tr>
<td><strong>Direct Permanent Investment</strong></td>
<td><strong>$ 70,382,318</strong></td>
</tr>
<tr>
<td><strong>Total Depreciable Capital</strong></td>
<td></td>
</tr>
<tr>
<td>Cost of Contingencies &amp; Contractor Fees</td>
<td>$ 12,668,817</td>
</tr>
<tr>
<td><strong>Total Depreciable Capital</strong></td>
<td><strong>$ 83,051,135</strong></td>
</tr>
<tr>
<td><strong>Total Permanent Investment</strong></td>
<td></td>
</tr>
<tr>
<td>Cost of Land:</td>
<td>$ 1,661,023</td>
</tr>
<tr>
<td>Cost of Royalties:</td>
<td>$ -</td>
</tr>
<tr>
<td>Cost of Plant Start-Up:</td>
<td>$ 8,305,113</td>
</tr>
<tr>
<td><strong>Total Permanent Investment - Unadjusted</strong></td>
<td><strong>$ 93,017,271</strong></td>
</tr>
<tr>
<td>Site Factor</td>
<td>1.00</td>
</tr>
<tr>
<td><strong>Total Permanent Investment</strong></td>
<td><strong>$ 93,017,271</strong></td>
</tr>
</tbody>
</table>
10. OPERATING COST AND PROFITABILITY ANALYSIS
10.1 Operating Costs

The economic analysis of this project is based on results calculated using the Profitability Analysis Spreadsheet 4.0 provided by Seider et al [30]. A summary of the inputs specifications, assumptions, and operating timeline is shown below in Table 9.4.

Table 9.4: Summary of Base Case Profitability Analysis Input Summary

<table>
<thead>
<tr>
<th>General Information</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Process Title:</td>
<td>Fluidized Catalytic Cracking to Convert Biomass to Fuels- Base Case</td>
</tr>
<tr>
<td>Product:</td>
<td>BTX</td>
</tr>
<tr>
<td>Plant Site Location:</td>
<td>Louisiana</td>
</tr>
<tr>
<td>Site Factor:</td>
<td>1.00</td>
</tr>
<tr>
<td>Operating Hours per Year:</td>
<td>7919</td>
</tr>
<tr>
<td>Operating Days Per Year:</td>
<td>330</td>
</tr>
<tr>
<td>Operating Factor:</td>
<td>0.9040</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Product Information</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>This Process will Yield</td>
<td></td>
</tr>
<tr>
<td>2,194 kg of BTX per hour</td>
<td></td>
</tr>
<tr>
<td>52,659 kg of BTX per day</td>
<td></td>
</tr>
<tr>
<td>17,375,213 kg of BTX per year</td>
<td></td>
</tr>
<tr>
<td>Price</td>
<td>$1.10 /kg</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Chronology</th>
<th>Distribution of Permanent Investment</th>
<th>Production Capacity</th>
<th>Depreciation 5 year MACRS</th>
<th>Product Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>Year</td>
<td>Action</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2014</td>
<td>Design</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2015</td>
<td>Construction</td>
<td>100%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2016</td>
<td>Production</td>
<td>0%</td>
<td>45.0%</td>
<td>20.00%</td>
</tr>
<tr>
<td>2017</td>
<td>Production</td>
<td>0%</td>
<td>67.5%</td>
<td>32.00%</td>
</tr>
<tr>
<td>2018</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>19.20%</td>
</tr>
<tr>
<td>2019</td>
<td>Production</td>
<td>90.0%</td>
<td>11.52%</td>
<td>1.17</td>
</tr>
<tr>
<td>2020</td>
<td>Production</td>
<td>90.0%</td>
<td>11.52%</td>
<td>1.19</td>
</tr>
<tr>
<td>2021</td>
<td>Production</td>
<td>90.0%</td>
<td>5.76%</td>
<td>1.21</td>
</tr>
<tr>
<td>2022</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.24</td>
</tr>
<tr>
<td>2023</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.26</td>
</tr>
<tr>
<td>2024</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.29</td>
</tr>
<tr>
<td>2025</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.31</td>
</tr>
<tr>
<td>2026</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.34</td>
</tr>
<tr>
<td>2027</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.37</td>
</tr>
<tr>
<td>2028</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.40</td>
</tr>
<tr>
<td>2029</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.42</td>
</tr>
<tr>
<td>2030</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td>1.45</td>
</tr>
</tbody>
</table>
10.1.1 Variable Costs

The variable costs of this plant are accrued through general expenses, raw materials, and utilities. In addition, the revenue generated from the by-product of electricity is included in the variable costs, as summarized in Table 10.1. Electricity is produced at a rate of 345 GWh per year and assumed to be sold at the average Louisiana electricity price of $.07/kWh. After accounting for the plant’s electricity requirements, the revenue generated by electricity amounts to $3.5 MM/yr. The variable costs for this plant sum to approximately $32 MM.

Table 10.1: Summary of Base Case Annual Variable Costs

<table>
<thead>
<tr>
<th>Variable Cost Summary</th>
<th>Variable Costs at 100% Capacity:</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Expenses</td>
<td></td>
</tr>
<tr>
<td>Selling / Transfer Expenses</td>
<td>$573,382</td>
</tr>
<tr>
<td>Direct Research</td>
<td>$917,411</td>
</tr>
<tr>
<td>Allocated Research</td>
<td>$95,564</td>
</tr>
<tr>
<td>Administrative Expense</td>
<td>$382,255</td>
</tr>
<tr>
<td>Management Incentive Compensation</td>
<td>$238,909</td>
</tr>
<tr>
<td><strong>Total General Expenses</strong></td>
<td><strong>$2,207,521</strong></td>
</tr>
<tr>
<td>Raw Materials</td>
<td>$1.900869 per kg of BTX</td>
</tr>
<tr>
<td></td>
<td>$33,028,000</td>
</tr>
<tr>
<td>Byproducts</td>
<td>$0.201394 per kg of BTX</td>
</tr>
<tr>
<td></td>
<td>($3,499,256)</td>
</tr>
<tr>
<td>Utilities</td>
<td>$0.025592 per kg of BTX</td>
</tr>
<tr>
<td></td>
<td>$444,662</td>
</tr>
<tr>
<td><strong>Total Variable Costs</strong></td>
<td><strong>$32,180,927</strong></td>
</tr>
</tbody>
</table>

General expenses cover the costs associated with sales, research, administration, and management. Because this process applies a relatively new technology, a significant amount of capital costs will need to be allocated toward research. The direct and allocated research costs were subsequently set at 4.8% and .5% of sales, respectively.
The raw materials used in this plant are biomass in the form of woodchips and a ZSM-5 catalyst. The purchase price of the biomass is taken as $40/ton, which accounts for transportation of the woodchips, and 400,000 metric ton/yr is required for the process input. At least ten counties in the southwestern portion of Louisiana produces more than 100,000 metric ton per year of biomass. Therefore, this process uses approximately 40% of the forest biomass available in the southwestern region of Louisiana. The second raw material cost is accrued from the purchase of the zeolite catalyst, which can be purchased at $10/kg. This process requires approximately 1.7 million kg of catalyst per year, resulting in a variable cost of $17 MM.

Utilities account for a significant portion of expenses in this process, as discussed in Section 6 of this report. The utility costs for boiler-feed water and chilled water were obtained from Seider et al. and were taken as $0.000476/kg and $4.0/GJ, respectively [30].

10.1.2 Fixed Costs

Fixed costs are those costs incurred by the project regardless of yield of BTX produced. Such costs include salaries and benefits, maintenance, operating overhead, taxes, and insurance. The fixed costs sum to $12.6 MM, as summarized in Table 10.2.
Table 10.2: Summary of Base Case Annual Fixed Costs

<table>
<thead>
<tr>
<th>Fixed Cost Summary</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operations</strong></td>
<td></td>
</tr>
<tr>
<td>Direct Wages and Benefits</td>
<td>$416,000</td>
</tr>
<tr>
<td>Direct Salaries and Benefits</td>
<td>$62,400</td>
</tr>
<tr>
<td>Operating Supplies and Services</td>
<td>$24,960</td>
</tr>
<tr>
<td>Technical Assistance to Manufacturing</td>
<td>$300,000</td>
</tr>
<tr>
<td>Control Laboratory</td>
<td>$325,000</td>
</tr>
<tr>
<td><strong>Total Operations</strong></td>
<td><strong>$1,128,360</strong></td>
</tr>
<tr>
<td><strong>Maintenance</strong></td>
<td></td>
</tr>
<tr>
<td>Wages and Benefits</td>
<td>$3,737,301</td>
</tr>
<tr>
<td>Salaries and Benefits</td>
<td>$934,325</td>
</tr>
<tr>
<td>Materials and Services</td>
<td>$3,737,301</td>
</tr>
<tr>
<td>Maintenance Overhead</td>
<td>$186,865</td>
</tr>
<tr>
<td><strong>Total Maintenance</strong></td>
<td><strong>$8,595,792</strong></td>
</tr>
<tr>
<td><strong>Operating Overhead</strong></td>
<td></td>
</tr>
<tr>
<td>General Plant Overhead:</td>
<td>$365,652</td>
</tr>
<tr>
<td>Mechanical Department Services:</td>
<td>$123,601</td>
</tr>
<tr>
<td>Employee Relations Department:</td>
<td>$303,852</td>
</tr>
<tr>
<td>Business Services:</td>
<td>$381,102</td>
</tr>
<tr>
<td><strong>Total Operating Overhead</strong></td>
<td><strong>$1,174,206</strong></td>
</tr>
<tr>
<td><strong>Property Taxes and Insurance</strong></td>
<td></td>
</tr>
<tr>
<td>Property Taxes and Insurance:</td>
<td>$1,661,023</td>
</tr>
<tr>
<td><strong>Other Annual Expenses</strong></td>
<td></td>
</tr>
<tr>
<td>Rental Fees (Office and Laboratory Space):</td>
<td>$-</td>
</tr>
<tr>
<td>Licensing Fees:</td>
<td>$-</td>
</tr>
<tr>
<td>Miscellaneous:</td>
<td>$-</td>
</tr>
<tr>
<td><strong>Total Other Annual Expenses</strong></td>
<td>$-</td>
</tr>
<tr>
<td><strong>Total Fixed Costs</strong></td>
<td><strong>$12,559,381</strong></td>
</tr>
</tbody>
</table>
10.1.3 Working Capital

Working capital is the sum of the accounts receivable, cash reserves, inventory, and raw materials minus the accounts payable. The time period for accounts payable and receivable was taken as 30 days each. The inventory of raw materials and BTX was taken as 1 day and 1 month, respectively. In combination with a total permanent investment of $93 MM and the working capital, the total capital investment is $95 MM, as summarized in Table 10.3.

Table 10.3: Summary of Base Case Working Capital

<table>
<thead>
<tr>
<th>Working Capital</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accounts Receivable</td>
<td>$ 706,909</td>
<td>$ 353,455</td>
<td>$ 353,455</td>
</tr>
<tr>
<td>Cash Reserves</td>
<td>$ 480,971</td>
<td>$ 240,486</td>
<td>$ 240,486</td>
</tr>
<tr>
<td>Accounts Payable</td>
<td>$(1,238,030)</td>
<td>$(619,015)</td>
<td>$(619,015)</td>
</tr>
<tr>
<td>BTX Inventory</td>
<td>$ 23,564</td>
<td>$ 11,782</td>
<td>$ 11,782</td>
</tr>
<tr>
<td>Raw Materials</td>
<td>$ 1,221,584</td>
<td>$ 610,792</td>
<td>$ 610,792</td>
</tr>
<tr>
<td>Total</td>
<td>$ 1,194,998</td>
<td>$ 597,499</td>
<td>$ 597,499</td>
</tr>
</tbody>
</table>

Present Value at 10%  

| Present Value at 10% | $ 1,086,362 | $ 493,801 | $ 448,910 |

Total Capital Investment  

| Total Capital Investment | $95,046,343 |

10.2 Profitability Analysis

10.2.1 Base Case

The project’s profitability is based on various factors including the return on investment (ROI), investor’s rate of return (IRR), and net present value (NPV). Base and best case scenarios for this project were analyzed at a discount rate of 10% and a production lifetime of 15 years. In the base case scenario, the process yield of approximately 17 MM kg of BTX per year at a sale price of $1.1/kg was used. The base case profitability analysis resulted in a ROI is -20 % and a NPV of $(157) MM, with a negative IRR all sensitivities. The cash flow summary and NPV calculations are summarized in Table 10.3 and the profitability measures in Table 10.4.
### Table 10.3: Base Case Cash Flow Summary

<table>
<thead>
<tr>
<th>Year</th>
<th>Percentage of Design Capacity</th>
<th>Product Unit Price</th>
<th>Sales</th>
<th>Capital Costs</th>
<th>Working Capital</th>
<th>Var Costs</th>
<th>Fixed Costs</th>
<th>Depreciation</th>
<th>Allowance</th>
<th>Taxable Income</th>
<th>Taxes</th>
<th>Net Earnings</th>
<th>Cash Flow</th>
<th>Cumulative Net Present Value at 10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014</td>
<td>0%</td>
<td>$1.10</td>
<td>8,600,700</td>
<td>(93,017,300)</td>
<td>(1,195,000)</td>
<td>(14,481,400)</td>
<td>(12,569,400)</td>
<td>(16,610,200)</td>
<td>-</td>
<td>(35,050,300)</td>
<td>12,968,600</td>
<td>(22,081,700)</td>
<td>(6,098,000)</td>
<td>(94,128,300)</td>
</tr>
<tr>
<td>2015</td>
<td>0%</td>
<td>$1.12</td>
<td>13,159,100</td>
<td>(597,900)</td>
<td>(21,722,100)</td>
<td>(12,569,400)</td>
<td>(26,574,400)</td>
<td>-</td>
<td>(47,098,800)</td>
<td>17,648,500</td>
<td>(30,050,200)</td>
<td>(4,071,300)</td>
<td>(93,722,100)</td>
<td></td>
</tr>
<tr>
<td>2016</td>
<td>46%</td>
<td>$1.14</td>
<td>17,996,400</td>
<td>(38,962,800)</td>
<td>(15,945,800)</td>
<td>(12,569,400)</td>
<td>(9,987,500)</td>
<td>(32,695,400)</td>
<td>12,149,100</td>
<td>(20,689,300)</td>
<td>(11,199,800)</td>
<td>(106,792,400)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2017</td>
<td>90%</td>
<td>$1.17</td>
<td>18,619,400</td>
<td>(38,962,800)</td>
<td>(12,569,400)</td>
<td>(9,987,500)</td>
<td>(32,470,300)</td>
<td>12,014,000</td>
<td>(20,486,300)</td>
<td>(10,888,800)</td>
<td>(11,908,800)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2018</td>
<td>90%</td>
<td>$1.21</td>
<td>18,991,800</td>
<td>(38,962,800)</td>
<td>(12,569,400)</td>
<td>(4,783,700)</td>
<td>-</td>
<td>(27,314,200)</td>
<td>10,106,200</td>
<td>(17,207,900)</td>
<td>(12,434,200)</td>
<td>(119,284,400)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2019</td>
<td>90%</td>
<td>$1.24</td>
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### Table 10.4: Base Case Profitability Measures

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10.2.2 Sensitivity Analysis

The sensitivity analysis of the base case changes the price of BTX with the variable costs accrued annually from plant operation. The price of BTX has recently fallen to as low as $.75/kg in January of 2015, but at its peak in August of 2014, BTX was selling at $1.54/kg. BTX generally sells at double the price of crude oil, but the market for crude oil has fallen drastically since the summer of 2014. Economic analysts predict the price of BTX to rise once again and stabilize, which may greatly affect the profitability of this plant. The base case analysis used a BTX sale price of $1.1/kg.

With plant production projected to begin in 2017, the price of BTX will have likely recovered to a healthy state, increasing the profitability potential of a BFCC plant such as the one proposed in this report. To account for the fluctuations in BTX prices, the IRR was analyzed at a BTX range of $.55/kg to $1.65/kg, which represents ± 50% of the base case value.

The variable costs of this plant are likely to vary considerably, as reflected by the fact that few industrial scale BFCC plants are currently in operation. The change in IRR was analyzed for variable costs ranging from $21 MM to $62 MM, which represents ± 50% of the base case value. A summary of the sensitivity analysis for the price of BTX and variable costs is shown in Table 10.5.
### Table 10.5: Base Case Sensitivity Analysis

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In this sensitivity analysis, all combinations of overestimates and underestimates in the variable costs and sale price of BTX result in a negative IRR projection. The result of this sensitivity sheds light on the dependence of BTX yield and utility costs on the profitability potential of this project. Due to the large amount of vapor streams in this process, high electricity costs are accrued for the movement and pressurization of these streams throughout the plant. It is also important to note that the yield of BTX was based off a theoretical study, and in practice double the yield of BTX could likely be achieved.

10.2.2 Best Case

In the best case scenario, the yield of BTX was doubled, which may be achieved on industrial scales, at a sale price of $1.54/kg, which is possible when the market is strong. In addition, a renewable fuel credit of $1.01/gal was incorporated into the best case analysis. These assumptions resulted in a ROI of 81%, an IRR is 70%, and a NPV of $506 MM. The cash flow summary and NPV calculations for this best case scenario are summarized in Table 10.6.
Table 10.6: Best Case Cash Flow Summary

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<th>Price</th>
<th>Sales</th>
<th>Capital Costs</th>
<th>Working Capital</th>
<th>Var Costs</th>
<th>Fixed Costs</th>
<th>Depreciation</th>
<th>Net Earnings</th>
<th>Cash Flow</th>
<th>Cumulative Net Present Value at 10%</th>
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<td>68%</td>
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11. OTHER IMPORTANT CONSIDERATIONS
11.1 Plant Startup

Plant startup will require particular attention due to the extensive heat network and large amount of utilities required throughout the process. The startup of the reactor will be especially important, as the temperature must reach 600 °C in order to foster the formation of desired aromatic products during catalytic fast pyrolysis. During startup, a natural gas fired heater will be needed to raise the temperature of the riser to within the range of pyrolysis. In addition, the purge stream of volatile products from the riser will be able to provide the required flowrate of carrier gas needed to obtain fluidization in the riser, but once steady state has been reached. Therefore, it is important that substantial fresh nitrogen be fed to the riser during startup to ensure that the fine biomass particles become fluidized.

11.2 Plant Control

Process control will be an important to ensuring cohesive plant operation. Specific areas of importance for process control will be monitoring the temperature in the circulating fluidized bed riser and catalytic regenerator. Flow control of the fluidized streams should also be areas of focus, as temperature may often be a function of flow rate. Finally, monitoring the pressure of the 3-phase liquid flash drum is of critical importance to ensuring the maximum output of valuable product from the process.

The circulating fluidized bed riser is the medium for the catalytic fast pyrolysis of biomass in the presence of a ZSM-5 catalyst. Pyrolysis occurs in the absence of oxygen at moderate pressures and a temperature range of 200-760 °C, producing syngas and coke. A similar process, gasification, occurs with very little oxygen between of 480-1700 °C. In order to prevent deactivation of the catalyst, which has an upper limit of 700 °C, and reduce the amount
of oxygenated products, the temperature of the riser must be controlled within the pyrolysis bounds.

Controlling the flow of the fluidized streams will be of great importance due to the high number of recycles and purges throughout the plant. Flow controls at the purge of the carrier gas as well as the catalyst purge will be integral to preventing buildup of unwanted streams in the system. The ratio of catalyst to biomass feed should be maintained at 4:1 to ensure conversion to the desired products. The total amount of carrier gas in the system should not deviate from the set point; a flow rate below the set point will not fluidized the solid biomass particles, causing reactor build up, while too high a flow rate will cause the biomass particles to be blown out the top devoid of catalyst contact. The flow of oxygen to the regenerator will also need particular attention so as not heat generate substantial heat to raise the outlet stream above 700 °C.

The flash drum can be operated at a number of different pressure and temperature combinations. A sensitivity analysis of the pressure and temperature conditions in the flash drum revealed that the extraction of valuable products is maximized at high pressures. However, high product yields are also obtained at more moderate pressures. Operating the flash drum at more moderate conditions reduces the operating costs associated with this extraction process. Therefore, control processes should be put in place to maintain the set points of the flash drum.

11.3 Plant Layout

The required equipment for the plant includes eight heat exchangers, six blowers, three compressors, three pumps with electric motors, two solid/vapor cyclones, two combustors, three hoppers, three dryers, three pulverizers, four screw feeders, two distillation columns, one 3 phase flash drum, one fluidized bed riser, one turbine, and pole sheds for long-term storage. The
capacity of each pole shed is 8000 ft² and should be able to store a one month supply of biomass for plant operation. The yearly input capacity of this process requires 800 MM pounds of dry biomass, which translate to 67 MM dry pounds of biomass for one month’s production capacity.

A majority of the plant’s layout will be attributed to solids handling, specifically the storage of the biomass. Pumps will be used to transport the cooling and process water used throughout the plant in the heat integrated steam co-generation scheme. Hoppers, which store one day’s worth of biomass input, will be gravity fed to the dryers. Screw feeders will be used to transport the solid biomass particles during plant operation and compressors will be placed between piping for the movement of vapors. Star valves will be used to remove solid particles from the bottoms of the two solid/vapor cyclones used throughout the process.

11.4 Plant Location

The operating costs of this process are sensitive to the availability of biomass and the proximity of customer refineries and chemical plants. Costs associated with the transportation of the biomass feedstock can be greatly mitigated with increasing proximity to the source. The distribution of biomass feedstock densities across the U.S., as shown in Figure 11.1, indicates a favorable plant location in the northwest and southeastern regions of the country. In addition, the wood biomass is available in the largest densities at $40/dry ton, although biomass can also be obtained from $20/dry ton and $60/dry ton but in less availability across the U.S.
There is also a high density of oil and gas refineries in the gulf coast region. Due to the high density of biomass feedstock as well as commercial customers in the gulf coast region, the optimal plant location was decided as Louisiana. As shown below in Figure 11.2, Louisiana has a high density of refineries (represented as green rectangles) in the southern portion of the state. Biomass feedstock can also be obtained from local sawmills in this region at a density capacity of 100 dry ton/square mile.
The Louisiana plant location will reduce operating costs and help optimize transportation logistics in both procuring the biomass and selling products to customers. The close proximity of the plant to the feedstock as well as the end user will therefore result in a more economical plant.

11.5 Environmental & Safety Considerations

This BFCC plant does not have a significant impact on the environment, although care should be taken to control emissions of greenhouse gases (GHGs). In addition, this process is renewable because the wood is naturally replenished by nature and is a non-food energy source. Biomass is organic material produced by the photosynthesis of light and carbon dioxide; its makeup of organic carbon compounds can be used to generate energy. The proximity of the plant to both biomass resources and customers minimizes the relative energy expenditure associated with construction and transportation as compared.
Special notice should be paid to the fact that there is a significant amount of carbon dioxide and carbon monoxide circulating in the system at steady-state. Most of these gases are combusted for their heating value, yet a small amount is still released from the system. Efforts were taken to minimize the release of GHGs from the system through a waste-heat boiler.

This process does produce some chemicals which are hazardous and require close monitoring during operation. In addition, some vapor streams are operated under pressure to facilitate transportation throughout the plant. Carbon monoxide, benzene, toluene, xylene, ethylbenzene, benzo furan are extremely flammable gases which can be toxic to humans if inhaled. Carbon dioxide may also become combustible when pressurized. More information on the hazards of each components are listed in the material safety data sheets of Appendix C.
12. CONCLUSIONS AND RECOMMENDATIONS
In summary, a process for the production of BTX from forest biomass has been designed and costed. In addition, base and best case profitability analyzes have been performed. The base case profitability analysis resulted in a negative NPV and ROI, even under a range of variable costs and product sale prices. The best case scenario assumed double the yield of BTX and a sale price of product in a healthy market, as well as renewable fuel credit. This best case scenario resulted in both a positive NPV and ROI, even for overestimated variable costs and underestimate product prices. The yield of BTX and the utility requirements associated with transporting the vapor streams have a large impact on the profitability of the plant. Moreover, the raw material requirements for the catalyst are much higher than are actually required in industrial FCC operation, thereby also having a large effect on the plant’s profitability.

We recommend that the base design for this process not be further pursued unless lab scale and pilot plant tests prove higher conversion rates of biomass to BTX. Another factor is the current decline in the BTX market- with BTX currently selling at approximately half the price it was in the summer of 2014, potential revenue for this project squanders expectations. Although the conversion of biomass to BTX may not be a desirable investment venture, biomass has a large heating value and can be burned directly for its energy content to generate electricity. As is done in coal-fired power plants, the revenue that could be generated from burning biomass alone to generate electricity is roughly $44 MM per year assuming a lower heating value of 19,000 kJ/kg, an electric power efficiency of 35%, and an electricity price of $.07/kWh.

Although this project may not prove feasible, technologies to convert biomass into more valuable products will likely gain focus as renewable energy develops into the main source for society’s energy demands.
13. ACKNOWLEDGEMENTS
We would like to especially thank Dr. Matthew Targett for conceptualizing this project and continually investing his time and energy into its development. Dr. Targett’s subject matter expertise, advice, and encouragement were integral in helping us successfully execute this design project. We would also like to thank Professor Leonard Fabiano and Dr. Talid Sinno for their continued assistance and engagement in our project. Finally, we would like to thank the industrial consultants who attended weekly design meetings and helped in solving the design challenges we encountered along the way.
14. REFERENCES


Appendix A: Sample Calculations

A.1 Fluidization Velocity of Carrier Gas

Properties:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carrier density (600 °C)</td>
<td>0.4</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Carrier viscosity (600 °C)</td>
<td>5.00E-07</td>
<td>kg/m·s</td>
</tr>
<tr>
<td>Catalyst density</td>
<td>720</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Catalyst diameter</td>
<td>0.002</td>
<td>m</td>
</tr>
<tr>
<td>Void fraction</td>
<td>0.45</td>
<td>-</td>
</tr>
<tr>
<td>Gravitational constant</td>
<td>9.8</td>
<td>m²/s²</td>
</tr>
</tbody>
</table>

Ergun equation: \[ g(\rho_s - \rho) = \frac{1.75\rho u^2}{d_p e^3} + \frac{150\mu(1-e)u}{d_p e^3} \]

\[ \frac{1.75 \times 4 \text{ kg/m}^3 \cdot u^2}{.002 \times (0.45)^3} + \frac{150 \times 5.0 \times 10^{-7} \text{ kg/m}^3 \cdot (1-0.45)u}{.002 m^2 \times (0.45)^3} - \left( 9.8 \text{ m/s}^2 \right) (720 - .4) \frac{\text{kg/m}^3}{m} = 0 \]

\[ \Rightarrow u = 1.34 \frac{m}{s} \]

Reynold’s number: \[ Re = \frac{\rho_d p u}{\mu} = \frac{4 \text{ kg/m}^3 \cdot .002 m \cdot 1.34 \frac{m}{s}}{5.0 \times 10^{-7} \text{ kg/m}^3} = 2,145 \]

Drag Coefficient: \[ C_D = \frac{18}{Re^{2/5}} = 0.18 \]

Entrainment velocity:

\[ u_e = \sqrt{\frac{4(\rho_s - \rho)gd_p}{3\rho C_D}} = \sqrt{\frac{4 \times (720 - .4) \text{ kg/m}^3 \cdot 9.8 \text{ m/s}^2 \cdot .002 m}{3 \cdot 4 \text{ kg/m}^3 \cdot 18}} = 16.14 \frac{m}{s} = 52.95 \frac{ft}{s} \]

For an average residence time of 2.5 s in the riser:

Height = \[ u_e \cdot \tau = 52.95 \frac{ft}{s} \times 2.5 \text{ s} = 132.4 \text{ ft} \]

Typical FCC Riser dimensions in range of \( u_e \) and \( \tau \): \( D = 2 \text{ ft}, H = 75 \text{ ft} \)

So, \( D = 132.4 \text{ ft} \times \frac{2 \text{ ft}}{75 \text{ ft}} = 3.5 \text{ ft} \)

Increase area needed by factor of 8 to account for ash and catalyst entering reactor:

\[ A_{cs} = \frac{\pi D^2}{4} \times 8 = 2\pi D^2 = 2\pi (.002 \text{ m})^2 = 78.29 \text{ ft}^2 = 7.27 \text{ m}^2 \]

Carrier flow rate required:

\[ \dot{m} = u_e \cdot A_{cs} = 16.14 \frac{m}{s} \times 7.27 \text{ m}^2 = 14,039.12 \frac{\text{kg}}{\text{hr}} \]
A.2 Vessel Sizing

A.2.1 Circulating Fluidized Bed Riser: R201

From fluidization of carrier gas calculations: \( u_t = 52.95 \text{ ft/s} \)

Let \( \tau = 2.5 \text{ s} \)

Height = \( u_t \cdot \tau = 52.95 \frac{\text{ft}}{\text{s}} \cdot 2.5 \text{ s} = 132.4 \text{ ft} \)

From typical sizing of FCC reactors: For \( H = 75 \text{ ft} \), \( D = 2 \text{ ft} \)

Diameter = \( 132.4 \text{ ft} \cdot \frac{2 \text{ ft}}{75 \text{ ft}} = 3.5 \text{ ft} \)

A.2.2 Solid/Vapor Cyclone: Cy-201

Properties:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor density</td>
<td>0.0004 g/cm³</td>
<td></td>
<td>Vapor Flowrate</td>
<td>52,001 kg/hr</td>
<td></td>
</tr>
<tr>
<td>Solid density</td>
<td>0.788 g/cm³</td>
<td></td>
<td>Solid Flowrate</td>
<td>7,635 kg/hr</td>
<td></td>
</tr>
<tr>
<td>Weighted Average density</td>
<td>0.105 g/cm³</td>
<td></td>
<td>Total Flowrate</td>
<td>59,637 kg/hr</td>
<td></td>
</tr>
</tbody>
</table>

\[
\begin{align*}
    u &= \sqrt{\frac{\rho_s - \rho_v}{\rho_v}} = \sqrt{\frac{(0.788 - 0.0004) \text{ g/cm}^3}{0.0004 \text{ g/cm}^3}} = 44.91 \text{ ft/s} \\
    \text{Area} &= \frac{52,001 \text{ kg/hr} \cdot 1000 \text{ g/1 kg} \cdot 0.000035314667 \text{ ft}^3/\text{cm}^3}{0.0004 \text{ g/cm}^3 \cdot 44.91 \frac{\text{ft}}{\text{s}} \cdot 3600 \frac{\text{s}}{1 \text{ hr}}} = 29.1 \text{ ft}^2 \\
    A_{cylinder+conical\ head} &= \pi \sqrt{h^2 + r^2} + 2\pi rh + \pi r^2 \\
    \text{Let } h &= 4D = 8r \\
    A_{cylinder+conical\ head} &= \pi \sqrt{64r^2 + r^2} + 16\pi r^2 + \pi r^2 = \pi r^2 (\sqrt{65} + 17) = 78.73r^2 \\
    \sqrt{\frac{A}{78.73}} &= \sqrt{\frac{29.1 \text{ ft}^2}{78.73}} = 0.61 \text{ ft} \\
    \text{Diameter} = 2r &= 1.2 \text{ ft.} \\
    \text{Height} &= 4D = 3.6 \text{ ft.}
\end{align*}
\]
A.2.3 Combustor: R-202

Properties:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor density</td>
<td>0.0023 g/cm³</td>
</tr>
<tr>
<td>Solid density</td>
<td>2.25 g/cm³</td>
</tr>
<tr>
<td>Weighted Average density</td>
<td>0.045 g/cm³</td>
</tr>
<tr>
<td>Vapor Flowrate</td>
<td>390,859 kg/hr</td>
</tr>
<tr>
<td>Solid Flowrate</td>
<td>7,627 kg/hr</td>
</tr>
<tr>
<td>Total Flowrate</td>
<td>398,486 kg/hr</td>
</tr>
</tbody>
</table>

\[
u = \sqrt{\frac{\rho_s - \rho_v}{\rho_v}} = \sqrt{\frac{(2.25 - 0.0023) \frac{g}{cm^3}}{0.0023 \frac{g}{cm^3}}} = 31.23 \text{ ft/s}
\]

\[
\text{Area} = \frac{\rho_s \cdot 1000 \frac{g}{1 \text{ kg}} \cdot 0.000035314667 \frac{ft^3}{cm^3}}{0.0023 \frac{g}{cm^3} \cdot 31.23 \frac{ft}{s} \cdot 3600 \frac{s}{1 \text{ hr}}} = 53.17 \text{ ft}^2
\]

\[
D = \frac{4 \cdot A_{cs}}{\pi} = \frac{4 \cdot 53.17 \text{ ft}^2}{\pi} = 8.23 \text{ ft.}
\]

\[H = 3D = 24.69 \text{ ft.}\]

A.2.4 Solid/Vapor Cyclone: Cy-202

Properties:

<table>
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<th>Property</th>
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<tr>
<td>Vapor density</td>
<td>0.0036 g/cm³</td>
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<td>Solid density</td>
<td>5.4 g/cm³</td>
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<td>Weighted Average density</td>
<td>1.08 g/cm³</td>
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<tr>
<td>Vapor Flowrate</td>
<td>398,486 kg/hr</td>
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<tr>
<td>Solid Flowrate</td>
<td>99,474 kg/hr</td>
</tr>
<tr>
<td>Total Flowrate</td>
<td>497,960 kg/hr</td>
</tr>
</tbody>
</table>

\[
u = \sqrt{\frac{\rho_s - \rho_v}{\rho_v}} = \sqrt{\frac{(5.4 - 0.0036) \frac{g}{cm^3}}{0.0036 \frac{g}{cm^3}}} = 2.10 \frac{ft}{s}
\]

\[
\text{Area} = \frac{\rho_s \cdot 1000 \frac{g}{1 \text{ kg}} \cdot 0.000035314667 \frac{ft^3}{cm^3}}{0.0036 \frac{g}{cm^3} \cdot 2.10 \frac{ft}{s} \cdot 3600 \frac{s}{1 \text{ hr}}} = 5,127.92 \text{ ft}^2
\]

\[A_{cylinder+conical head} = \pi \sqrt{64r^2 + r^2} + 16\pi r^2 + \pi r^2 = \pi r^2(\sqrt{65} + 17) = 78.73r^2\]
\[
r = \sqrt{\frac{A}{78.73}} = \sqrt{\frac{5,127.92 \, \text{ft}^2}{78.73}} = 8.24 \, \text{ft}
\]
Diameter = 2r = 16.48 ft.

Height = 4D = 49.42 ft.

A.2.5 Three-Phase Flash Drum: Fl-301

Properties:

<table>
<thead>
<tr>
<th></th>
<th>.924</th>
<th>g/cm³</th>
<th>Organic Flowrate</th>
<th>3.076</th>
<th>kg/hr</th>
<th>Organic MW</th>
<th>.0896</th>
<th>kg/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Organic density</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aqueous density</td>
<td>.976</td>
<td>g/cm³</td>
<td>Aqueous Flowrate</td>
<td>9.013</td>
<td>kg/hr</td>
<td>Aqueous MW</td>
<td>.01802</td>
<td>kg/mol</td>
</tr>
<tr>
<td>Weighted Liquid density</td>
<td>.963</td>
<td>g/cm³</td>
<td>Liquid Flowrate</td>
<td>12.089</td>
<td>kg/hr</td>
<td>Liquid MW</td>
<td>.036</td>
<td>kg/mol</td>
</tr>
<tr>
<td>Volatile density</td>
<td>.015</td>
<td>g/cm³</td>
<td>Volatile Flowrate</td>
<td>39.912</td>
<td>kg/hr</td>
<td>Volatile MW</td>
<td>.0301</td>
<td>kg/mol</td>
</tr>
</tbody>
</table>

\[
F_{lv} = \frac{Q_l \cdot MW_l}{Q_v \cdot MW_v} \sqrt{\frac{\rho_v}{\rho_l}} = \frac{12,089 \, \text{kg/hr} \cdot .036 \, \text{kg/mol}}{39,912 \, \text{kg/hr} \cdot .0301 \, \text{kg/mol}} \sqrt{\frac{.015 \, \text{g/cm}^3}{.963 \, \text{g/cm}^3}} = .045
\]

\[
\ln (F_{lv}) = -3.09
\]

\[
K_{drum} = e^{(-1.8775 - .8146 \cdot F_{lv} - .1871 \cdot F_{lv}^2 - .0145 \cdot F_{lv}^3 - .001 \cdot F_{lv}^4)} = .445
\]

\[
u = K_{drum} \sqrt{\frac{\rho_l - \rho_v}{\rho_v}} = .447 \sqrt{\frac{(.963 - .015) \, \text{g/cm}^3}{.015 \, \text{g/cm}^3}} = 3.56 \, \text{ft/s}
\]

\[
A_{cs} = \frac{Q_v}{u \cdot \rho_v} = \frac{39,912 \, \text{kg/hr} \cdot 1000 \, \text{g/kg}}{3.56 \, \text{ft/s} \cdot .015 \, \text{g/cm}^3 \cdot 3600 \, \text{s/hr} \cdot (30.5 \, \text{cm})^3} = 7.42 \, \text{ft}^2
\]

\[
D = \sqrt{\frac{4 \cdot A_{cs}}{\pi}} = \sqrt{\frac{4 \cdot 7.42 \, \text{ft}^2}{\pi}} = 3.07 \, \text{ft}
\]

H = 3D = 9.22 ft.
A.2.6 Combustor: R-401

Properties:

<table>
<thead>
<tr>
<th></th>
<th>Density</th>
<th>Flowrate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor 1</td>
<td>.00094</td>
<td>398,486</td>
</tr>
<tr>
<td>Vapor 2</td>
<td>.012</td>
<td>26,192</td>
</tr>
<tr>
<td>Vapor 3</td>
<td>.0073</td>
<td>41.41</td>
</tr>
<tr>
<td>Vapor 4</td>
<td>.0016</td>
<td>424,720</td>
</tr>
<tr>
<td>Liquid</td>
<td>.706</td>
<td>702.13</td>
</tr>
</tbody>
</table>

\[
u = \sqrt{\frac{\rho_s - \rho_v}{\rho_v}} = \sqrt{\frac{.706 - .0016}{.0016}} \text{ g/cm}^3 = 20.85 \text{ ft/s}
\]

\[
\text{Area} = \frac{424,720 \text{ kg/hr} \cdot 1000 \text{ g/1 kg} \cdot 0.000035314667 \text{ ft}^3/\text{cm}^3}{.0016 \text{ g/cm}^3 \cdot 20.85 \text{ ft/s} \cdot 3600 \text{ s/1 hr}} = 123.1 \text{ ft}^2
\]

\[
D = \sqrt{\frac{4 \cdot A_{cs}}{\pi}} = \sqrt{\frac{4 \cdot 123.1 \text{ ft}^2}{\pi}} = 12.52 \text{ ft.}
\]

\[H = 3D = 37.56 \text{ ft.}\]
Appendix B: Aspen Results

B.1 Process Flow Diagram
B.2 Input Summary

DYNAMICS
DYNAMICS RESULTS=ON

TITLE 'Pyrolysis'

IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar & INVERSE-PRES='1/bar'

DEF-STREAMS MIXCIPSD ALL

SIM-OPTIONS MASS=BAL-CHE=YES FREE-WATER=NO OPER-YEAR=330. & UTL-REQD=YES

MODEL-OPTION

DATABANKS 'APV86 PURE32' / 'APV86 AQUEOUS' / 'APV86 SOLIDS' / 'APV86 INORGANIC' / 'APV86 ASPENPCD' / 'APV86 BIODIESEL' / 'APV86 COMBUST' / 'APV86 POLYMER' / 'APV86 ELECPURE' / 'APV86 EOS-LIT' / 'APV86 ETHYLENE' / 'APV86 HYSYS' / 'APV86 INITIATO' / 'APV86 NRTL-SAC' / 'APV86 PC-SAFT' / 'APV86 POLYPCSF' / 'APV86 SEGMENT' / 'FACTV86 FACTPCD' / 'NISTV86 NIST-TRC' / 'APV86 PURE20' / 'APV86 PURE22' / 'APV86 PURE24' / 'APV86 PURE25' / 'APV86 PURE26' / 'APV86 PURE27' / 'APV86 PURE28'

PROP-SOURCES 'APV86 PURE32' / 'APV86 AQUEOUS' / 'APV86 SOLIDS' / 'APV86 INORGANIC' / 'APV86 ASPENPCD' / 'APV86 BIODIESEL' / 'APV86 COMBUST' / 'APV86 POLYMER' / 'APV86 ELECPURE' / 'APV86 EOS-LIT' / 'APV86 ETHYLENE' / 'APV86 HYSYS' / 'APV86 INITIATO' / 'APV86 NRTL-SAC' / 'APV86 PC-SAFT' / 'APV86 POLYPCSF' / 'APV86 SEGMENT' / 'FACTV86 FACTPCD' / 'NISTV86 NIST-TRC' / 'APV86 PURE20' / 'APV86 PURE22' / 'APV86 PURE24' / 'APV86 PURE25' / 'APV86 PURE26' / 'APV86 PURE27' / 'APV86 PURE28'

COMPONENTS


CISOLID-COMPS CARBO-03 CELLO-01 DIPHE-01 GAIA-01 ALUMI-01

MOIST-COMPS WATER

SOLVE
RUN-MODE MODE=SIM

FLOWSHEET

BLOCK RYIELD IN=DRY-BIO OUT=S-V-PROD
BLOCK CYCLONE IN=S2 OUT=VAP-PROD COKECAT1
BLOCK HEATX1 IN=VAP-PROD S3 OUT=VAP-PROD2 STEAM
BLOCK RSTOIC IN=COKECAT2 S8 OUT=CAT+FLUE HEAT
BLOCK CYCLONE2 IN=S10 OUT=FLUE REGENCAT
BLOCK DRYER IN=WET-BIO DRY-AIR2 OUT=DRY-BIO WET-AIR
BLOCK FLASH3 IN=VAP-PRO3 OUT=VOLATILE ORGANIC AQUEOUS
BLOCK MIX2 IN=FRESHCAT REGENCAT OUT=CATFEED
BLOCK HEATER2 IN=CAT+FLUE HEAT OUT=CATFLUE2
PROP
PROPERTIES SRK FREE WATER=STEAMNBS

PROPERTY=UNIQUAC

PROP-DATA REVIEW-1
IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T-C PDROP=bar & INVERSE-PRES='1/bar'
PROP-LIST CHARGE
PVAL BENZO=01 0

PROP-DATA REVIEW-1
IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T-C & MOLE-ENTHALP='J/kmol' PDROP=bar INVERSE-PRES='1/bar'
PROP-LIST DHEFORM
PVAL BENZO=01 46.48

PROP-DATA REVIEW-1
IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T-C & MOLE-ENTHALP='kJ/mol' PDROP=bar INVERSE-PRES='1/bar'
PROP-LIST DHVLTD
PVAL BENZO=01 46.48 1.018264 -0.8747635 0.2916512 681 & 4 215 681

; TDE Aly-Lee ideal gas Cp
; "Heat capacity (Ideal gas )"

PROP-DATA CPIALE-1
IN-UNITS MET MOLE=HEAT-CA='J/kmol-K' PRESSURE=bar & TEMPERATURE-K DELTA-T-C PDROP=bar INVERSE-PRES='1/bar'
PROP-LIST CPIALEE
PVAL BENZO=01 51392.52 173867.4 543.8121 154951.2 1487.629 & 0 8.31447 200 1000
PVAL CARBO=03 20780.96 3930.973 -6957.123 71465.82 9.96575 & 0 8.31447 50 5000

; TDE equation for liquid Cp
; "Heat capacity (Liquid vs. Gas )"

PROP-DATA CPTLDE-1
IN-UNITS MET MOLE=HEAT-CA='J/kmol-K' PRESSURE=bar & TEMPERATURE-K DELTA-T-C PDROP=bar INVERSE-PRES='1/bar'
PROP-LIST CPTLDECS
PVAL BENZO=01 112731.8 91.02334 0.5151943 & -0.0004995536 & 5098.247 681 4 250 667.38

; TDE Watson equation for heat of vaporization
; "Enthalpy of vaporization or sublimation (Liquid vs. Gas )"

PROP-DATA DHVLTD-1
IN-UNITS MET PRESSURE=bar TEMPERATURE-K DELTA-T-C & MOLE-ENTHALP='J/kmol' PDROP=bar INVERSE-PRES='1/bar'
PROP-LIST DHVLTDEN
PVAL BENZO=01 18.11711 1.018264 -0.8747635 0.2916512 681 & 4 215 681

; TDE expansion for liquid molar density
; "Density (Liquid vs. Gas )"
PROP-DATA DNLEXS-1
  IN-UNITS MET PRESSURE=bar TEMPERATURE=K DELTA-T=C &
  MOLE-DENSITY='kmol/cum' PDROP=bar INVERSE-PRES='1/bar'
  PROP-LIST DNLEXSAT
  PVAL BENZO-01 2.896047 6.093528 2.060561 -0.4075595 &
  0.7211226 0 0 681 6 210 681

;ThermoML polynomials for liquid thermal conductivity
; "Thermal conductivity (Liquid vs. Gas )"

PROP-DATA KLTMLP-1
  IN-UNITS MET PRESSURE=bar TEMPERATURE=K &
  THERMAL-COND='Watt/m-K' DELTA-T=C PDROP=bar &
  INVERSE-PRES='1/bar'
  PROP-LIST KLTMLPO
  PVAL BENZO-01 0.2388756 -0.002954164 0.0000004167486 &
  -5.076213E-10 4 200 610

;ThermoML polynomials for vapor thermal conductivity
; "Thermal conductivity (Gas )"

PROP-DATA MULPPD-1
  IN-UNITS MET PRESSURE=bar TEMPERATURE=K VISCOSITY='N-
  sec/sqm' &
  DELTA-T=C PDROP=bar INVERSE-PRES='1/bar'
  PROP-LIST MULPPDS9
  PVAL BENZO-01 0.00006206041 0.9257641 1.405136 770.0771 &
  -17.71301 270 680

;ThermoML polynomials for vapor viscosity
; "Viscosity (Gas )"

PROP-DATA MUVTML-1

IN-UNITS MET PRESSURE=bar TEMPERATURE=K VISCOSITY='N-
  sec/sqm' &
  DELTA-T=C PDROP=bar INVERSE-PRES='1/bar'
  PROP-LIST MUVTMLPO
  PVAL BENZO-01 -0.000000088423 0.0000000254990 -9.260589E-13 &
  -1.340261E-15 4 450 1020

;TDE Wagner 25 liquid vapor pressure
; "Vapor pressure (Liquid vs. Gas )"

PROP-DATA WAGN25-1
  IN-UNITS MET PRESSURE='N/sqm' TEMPERATURE=K DELTA-T=C &
  PDROP=bar INVERSE-PRES='1/bar'
  PROP-LIST WAGNER25
  PVAL BENZO-01 7.719693 1.992513 -2.743703 &
  3.353024 15.32357 681 210 681

PROP-DATA SRKKIJ-1
  IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C &
  INVERSE-PRES='1/bar'
  PROP-LIST SRKKIJ
  BPVAL BENZE-01 TOLUE-01 .0 200000000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL TOLUE-01 BENZE-01 .020000000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL BENZE-01 METHA-01 .0313391000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL METHA-01 BENZE-01 .0313391000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL TOLUE-01 ETHYL-02 .0283552000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL ETHYL-02 BENZE-01 .0283552000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL BENZE-01 CARBO-02 .0880600000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL CARBO-02 BENZE-01 .0880600000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL TOLUE-01 METHA-01 .0818031000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL METHA-01 TOLUE-01 .0818031000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL M-XYL-01 CARBO-02 .1010000000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL CARBO-02 M-XYL-01 .1010000000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL P-XYL-01 CARBO-02 .0967800000 0.0 0.0 &
  273.1500000 726.8500000
  BPVAL CARBO-02 P-XYL-01 .0967800000 0.0 0.0 &
  273.1500000 726.8500000
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<tr>
<th>Pressure (bar)</th>
<th>Temperature (°C)</th>
<th>Delta T (°C)</th>
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<td>330.02</td>
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<tr>
<td>273.15</td>
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**Notes:**
- Units: bar, °C, bar
- Data was obtained from a database.
- The table provides pressure, temperature, and delta temperature values.
<table>
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<tr>
<th>Compound 1</th>
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<tr>
<td>XYL</td>
<td>TOLUE</td>
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</tr>
<tr>
<td>PHENO</td>
<td>M</td>
<td>O</td>
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<tr>
<td>ETHYL</td>
<td>1:3</td>
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</tr>
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</tr>
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</table>
BPVAL 1:3-B=01 1-BUT=01 0.0 24.23180000 0.0 0.0 & 51.00000000 51.00000000 0.0
DEF-SUBS-ATTR PSD PSD
IN-UNITS ENG
INTERVALS 2
SIZE-LIMITS 0.01 <mm> / 0.1 <mm> / 0.2 <mm>

STREAM AIR-IN
SUBSTREAM MIXED TEMP=25.00000000 PRES=1.000000000 &
MASS-FLOW=22193.846
MOLE-FRAC NITROGEN 0.79 / OXYGEN 0.21

STREAM CW1
SUBSTREAM MIXED TEMP=0. PRES=1. <atm> MASS-FLOW=55000.
MASS-FRAC WATER 1.

STREAM DRY-AIR
SUBSTREAM MIXED TEMP=25. PRES=1.013250000 MASS-FLOW=30000. &
FREE-WATER=NO NPHASE=1 PHASE=V
MOLE-FRAC AIR 1.

STREAM FRESHCAT
SUBSTREAM CIPSD TEMP=600. PRES=1. MASS-FLOW=215.86
MASS-FRAC ALUMO1 0.1
SUBS-ATTR PSD (0.5 0.5)
DEF-STREAMS HEAT HEAT
DEF-STREAMS HEAT HEAT2
DEF-STREAMS WORK ELECTRIC

BLOCK MIX1 MIXER
PARAM

BLOCK MIX2 MIXER
PARAM

BLOCK MIX3 MIXER
PARAM

BLOCK MIX4 MIXER
PARAM PRES=179.

BLOCK PURGE2 FSPLIT
FRAC N2PURGE 0.656252

BLOCK SPLIT1 FSPLIT
FRAC DEADCAT 0.00117

BLOCK HEATER2 HEATER
PARAM PRES=1.
UTILITY UTILITY ID=U-2

BLOCK HEATER3 HEATER
PARAM PRES=1. <atm>
UTILITY UTILITY ID=U-2

BLOCK FLASH3 FLASH3
PARAM TEMP=5. PRES=9.
UTILITY UTILITY ID=U-1

BLOCK HEATX1 HEATX
PARAM T-HOT=80.
FEEDS HOT-VAP-PROD COLD=S3
OUTLETS-HOT VAP-PROD2
OUTLETS-COLD STEAM
TQ-PARAM CURVE=YES

BLOCK HEATX2 HEATX
PARAM T=HOT=5.
FEEDS HOT=S11 COLD=S4
OUTLETS-HOT VAP=PRO3
OUTLETS-COLD CW2
TQ-PARAM CURVE=YES

BLOCK HEATX HEATX
PARAM T=COLD=600.
FEEDS HOT=COMGAS COLD=S12
OUTLETS-HOT N2PURGE2
OUTLETS-COLD NITRO-2
TQ-PARAM CURVE=YES

BLOCK HEATX4 HEATX
PARAM T=COLD=590.
FEEDS HOT=N2PURGE COLD=S13
OUTLETS-HOT N2PURGE2
OUTLETS-COLD NITRO-2
TQ-PARAM CURVE=YES

BLOCK HEATX5 HEATX
PARAM T=COLD=300.
FEEDS HOT=S11 COLD=S15
OUTLETS-HOT N2PURGE3
OUTLETS-COLD DRY-AIR2
TQ-PARAM CURVE=YES

BLOCK HEATX7 HEATX
PARAM T=COLD=480.
FEEDS HOT=N2PURGE COLD=S17
OUTLETS-HOT N2PURGE4
OUTLETS-COLD STEAM2
TQ-PARAM CURVE=YES

BLOCK HEATX8 HEATX
PARAM T=COLD=765.
FEEDS HOT=FLUE2 COLD=S6
OUTLETS-HOT FLUE3
OUTLETS-COLD STEAM3
TQ-PARAM CURVE=YES

BLOCK HEATX9 HEATX
PARAM T=COLD=540.
FEEDS HOT=GHG-2 COLD=S5
OUTLETS-HOT GHG-3
OUTLETS-COLD STEAM4
TQ-PARAM CURVE=YES

BLOCK DIST1 RADFRAC
PARAM NSTAGE=27 ALGORITHM=STANDARD MAXOL=25 DAMPING=NONE
COL-CONFIG CONDENSER=PARTIAL

FEEDS ORGANIC 13
PRODUCTS HIGHBOIL 27 L / DIST 1 V / BTX-MIX 1 L
P=SPEC 1 4.7 <atm>
COL-SPECs MASS=D:F=0.771728 DP-COL=3.7 <atm> MASS-
RR=0.713898 &
T1=30.
UTILITIES COND-UTIL=U-1 REB-UTIL=U-1

BLOCK DIST2 RADFRAC
PARAM NSTAGE=15 ALGORITHM=STANDARD MAXOL=50 DAMPING=NONE
COL-CONFIG CONDENSER=TOTAL

FEEDS S19 6
PRODUCTS PHENOL 15 L / BTX 1 L
P=SPEC 1 4.
COL-SPECs MASS=D:F=0.75 MASS-RR=0.75
SC-REFLUX OPTION=1
UTILITIES COND-UTIL=U-1 REB-UTIL=U-1

BLOCK COMBUST RSTOIC
PARAM TEMP=25. PRES=1. <atm>
STOIC 1 MIXED BENZE-01 -1. / OXYGEN -7.5 / CARBO-02 6. / &
WATER 3.
STOIC 2 MIXED TOLUE-01 -1. / OXYGEN -9. / CARBO-02 7. / &
WATER 4.
STOIC 3 MIXED ETHYL-01 -1. / OXYGEN -10.5 / CARBO-02 8. / &
WATER 5.
STOIC 4 MIXED M-XYL-01 -1. / OXYGEN -10.5 / CARBO-02 8. / &
WATER 5.
STOIC 5 MIXED P-XYL-01 -1. / OXYGEN -10.5 / CARBO-02 8. / &
WATER 5.
STOIC 6 MIXED O-XYL-01 -1. / OXYGEN -10.5 / CARBO-02 8. / &
WATER 5.
STOIC 7 MIXED STYRE-01 -1. / OXYGEN -10. / CARBO-02 8. / &
WATER 4.
STOIC 8 MIXED PHENO-01 -1. / OXYGEN -7. / CARBO-02 6. / &
WATER 3.
STOIC 9 MIXED INDEN-01 -1. / OXYGEN -11. / CARBO-02 9. / &
WATER 4.
STOIC 11 MIXED METHA-01 -1. / OXYGEN -2. / CARBO-02 1. / &
WATER 2.
STOIC 12 MIXED ETHYL-02 -1. / OXYGEN -3. / CARBO-02 2. / &
WATER 2.
STOIC 14 MIXED PROPY-01 -1. / OXYGEN -4.5 / CARBO-02 3. / &
WATER 3.
STOIC 15 MIXED 1-BUT-01 -1. / OXYGEN -6. / CARBO-02 4. / &
WATER 4.
STOIC 16 MIXED 1:3-B-01 -1. / OXYGEN -5.5 / CARBO-02 4. / &
WATER 3.
STOIC 17 MIXED BENZO-01 -1. / OXYGEN -9. / CARBO-02 8. / &
BLOCK RSTOIC
PARAM TEMP=600. PRES=179. EFF=0.88 DEFF=0.9 &
STOIC 1 MIXED CARBO-03 1. / OXYGEN =0.5 / CARBO-01 1.
STOIC 2 MIXED CARBO-03 -1. / OXYGEN =1. / CARBO-02 1.
UTILITY UTILITY-ID-U-2

BLOCK RYIELD
PARAM TEMP=600. PRES=179. EFF=0.88 DEFF=0.9 &
MOLE-YIELD MIXED BENZE-01 0.005810679 / TOLUE-01 &
0.006468288 / ETHYL-01 0.00022639 / M-XYL-01 &
0.00113195 / P-XYL-01 0.00113195 / O-XYL-01 &
0.000358451 / STYRE-01 0.000830097 / PHEN-01 &
0.001006178 / INDEN-01 0.001190644 / BENZO-01 &
0.000301853 / NAPHT-01 0.002218623 / METHA-01 &
0.001742753 / ETHYL-02 0.023064348 / PROPY-01 &
0.00025499 / 1-BUT-01 0.000534418 / 1:3-B-01 &
0.000406363 / CARBO-01 0.360852087 / CARBO-02 &
0.111136955 / CARBO-03 0.414362473 / CELLO-01 0. / &
WATER 0.327 / DIPHE-01 0. / GUAIA-01 0.
UTILITY UTILITY-ID-U-2

BLOCK-RSTOIC RSTOIC
PARAM TEMP=600. PRES=179. EFF=0.88 DEFF=0.9 &
STOIC 1 MIXED CARBO-03 1. / OXYGEN =0.5 / CARBO-01 1.
STOIC 2 MIXED CARBO-03 -1. / OXYGEN =1. / CARBO-02 1.
UTILITY UTILITY-ID-U-2

BLOCK P-1 PUMP
PARAM PRES=179. EFF=0.88 DEFF=0.9
UTILITY UTILITY-ID-U-1

BLOCK P-2 PUMP
PARAM PRES=179. EFF=0.88 DEFF=0.9
UTILITY UTILITY-ID-U-1

BLOCK P-3 PUMP
PARAM PRES=179. EFF=0.88 DEFF=0.9
UTILITY UTILITY-ID-U-1

BLOCK P-4 PUMP
PARAM DELP=45. <psi> EFF=0.88 DEFF=0.9
UTILITY UTILITY-ID-U-1

BLOCK P-5 PUMP
PARAM PRES=179. EFF=0.88 DEFF=0.9
UTILITY UTILITY-ID-U-1

BLOCK P-6 PUMP
PARAM DELP=25. <psi> EFF=0.88
UTILITY UTILITY-ID-U-2

BLOCK B-1 COMPR
PARAM TYPE=ISENTROPIC DELP=15. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1

BLOCK B-2 COMPR
PARAM TYPE=ISENTROPIC DELP=15. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1

BLOCK B-3 COMPR
PARAM TYPE=ISENTROPIC DELP=50. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1

BLOCK B-4 COMPR
PARAM TYPE=ISENTROPIC DELP=25. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1

BLOCK B-5 COMPR
PARAM TYPE=ISENTROPIC DELP=15. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001 MODEL-TYPE=COMPRESSOR
UTILITY UTILITY-ID-U-1

BLOCK B-7 COMPR
PARAM TYPE=ISENTROPIC DELP=25. <psi> SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1

BLOCK C-6 COMPR
PARAM TYPE=ISENTROPIC PRES=9. SEFF=0.88 MEFF=0.9 &
SB-MAXIT=30 SB-TOL=0.0001
UTILITY UTILITY-ID-U-1
BLOCK C-8 COMPR
  PARAM TYPE=ISENTROPIC DELP=40. <psi> SEFF=0.88 MEFF=0.9 &
  SB-MAXIT=30 SB-TOL=0.0001
  UTILITY UTILITY-ID=U-1

BLOCK C-9 COMPR
  PARAM TYPE=ISENTROPIC DELP=25. <psi> SEFF=0.88 MEFF=0.9 &
  SB-MAXIT=30 SB-TOL=0.0001
  UTILITY UTILITY-ID=U-1

BLOCK TURBINE COMPR
  PARAM TYPE=ISENTROPIC PRES=0.5 SEFF=0.88 MEFF=0.9 NPHASE=2 &
  SB-MAXIT=30 SB-TOL=0.0001
  MODEL TYPE=TURBINE
  BLOCK OPTION FREE-WATER=NO

BLOCK CYCLONE CYCLONE
  PARAM MODEL=SOLIDS-SEP TEMP=600. PRES=1.013250000
  SOLIDS-SEP SOLID=SPLIT=1. FLUID=SPLIT=1. CLASS=CHAR-SIZE

BLOCK CYCLONE2 CYCLONE
  PARAM MODEL=SOLIDS-SEP TEMP=700. PRES=1.000000000
  SOLIDS-SEP SOLID=SPLIT=1. FLUID=SPLIT=1. CLASS=CHAR-SIZE

BLOCK DRYER DRYER
  EXITMOIST WATER CIPSD 0.05
  OPERATION PRES=1.013250000 TEMP=175.
  UTILITY UTILITY-ID=U-1
  PARAM MOIST-BASIS=WET

BLOCK VALVE VALVE
  PARAM P-OUT=4.

UTILITY U-1 GENERAL
  COST ELEC-PRICE=0.07 <$/kWhr>
  PARAM UTILITY-TYPE-ELECTRICITY

UTILITY U-2 GENERAL
  COST ELEC-PRICE=0.07 <$/kWhr>
  PARAM UTILITY-TYPE-ELECTRICITY

DESIGN-SPEC AIRFEED
  DEFINE AIRTEMP STREAM-VAR STREAM-CARRIER2 SUBSTREAM-MIXED &
  VARIABLE-TEMP UOM="C"
  SPEC "AIRTEMP" TO "700"
  TOL-SPEC ".01"
  VARY STREAM-VAR STREAM-AIR-IN SUBSTREAM-MIXED &
  VARIABLE-MASS-FLOW UOM="kg/hr"
  LIMITS "0" "1000000"

DESIGN-SPEC N2FLOW
  DEFINE N2FLOW STREAM-VAR STREAM-CARRIER3 SUBSTREAM-MIXED &
  VARIABLE-STDEVOL-FLOW UOM="cum/hr"
  SPEC "N2FLOW" TO "106462"
  TOL-SPEC ".1"
  VARY BLOCK-VAR BLOCK-PURGE2 SENTENCE=FRAC VARIABLE=FRAC &
  ID1=N2PURGE
  LIMITS "0" ".99"

DESIGN-SPEC PURGE2
  DEFINE PURGE2 STREAM-VAR STREAM-CARRIER3 SUBSTREAM-MIXED &
  VARIABLE-MASS-FLOW UOM="kg/hr"
  SPEC "PURGE2" TO "13900"
  TOL-SPEC ".1"
  VARY BLOCK-VAR BLOCK-PURGE2 SENTENCE=FRAC VARIABLE=FRAC &
  ID1=N2PURGE
  LIMITS ".001" ".99"

DESIGN-SPEC PURGESPE
  DEFINE PURGE STREAM-VAR STREAM-CARRIER SUBSTREAM-MIXED &
  VARIABLE-TEMP UOM="C"
  SPEC "PURGE" TO "600"
  TOL-SPEC ".1"
  VARY BLOCK-VAR BLOCK-PURGE2 SENTENCE=FRAC VARIABLE=FRAC &
  ID1=N2PURGE
  LIMITS ".001" ".99"

DESIGN-SPEC STEAM2
  DEFINE STEAM2 STREAM-VAR STREAM-STEAM2 SUBSTREAM-MIXED &
  VARIABLE-TEMP UOM="C"
  SPEC "STEAM2" TO "540"
  TOL-SPEC ".01"
  VARY STREAM-VAR STREAM-WATER2 SUBSTREAM-MIXED &
  VARIABLE-MASS-FLOW UOM="kg/hr"
  LIMITS "0" "100000"

DESIGN-SPEC W2
  DEFINE W2 STREAM-VAR STREAM-STEAM SUBSTREAM-MIXED &
  VARIABLE-TEMP UOM="C"
  SPEC "W2" TO "200"
  TOL-SPEC ".1"
  VARY STREAM-VAR STREAM-WATER SUBSTREAM-MIXED &
  VARIABLE-MASS-FLOW UOM="kg/hr"
  LIMITS "0" "20000"

DESIGN-SPEC WATER
  DEFINE WATER STREAM-VAR STREAM-STEAM SUBSTREAM-MIXED &
  VARIABLE-TEMP UOM="C"
  SPEC "WATER" TO "200"
  TOL-SPEC ".1"
VARY MASS-FLOW STREAM=WATER SUBSTREAM=MIXED COMPONENT=WATER

\[ UOM="kg/hr" \]
\[ LIMITS "0" "5000000" \]

EO-CONV-OPTI

SENSITIVITY CARRIER

DEFINE CARRIERF STREAM-VAR STREAM=NITRO-2 SUBSTREAM=MIXED

\[ VARIABLE=STDVOL-FLOW UOM="l/hr" \]
\[ TABULATE 1 "1" \]
\[ TABULATE 2 "CARRIERF" \]

VARY MASS-FLOW STREAM=NITRO-1 SUBSTREAM=MIXED COMPONENT=NITROGEN UOM="kg/hr"

RANGE LOWER="1000" UPPER="40000" NPOINT="15"

CONV-OPTIONS

PARAM TOL=0.001
WEGSTEIN MAXIT=150

BLOCK-REPORT NEWPAGE

STREAM-REPORT MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

PROPERTY-REF NOPARAM-PLUS
DISABLE

SENSITIVITY CARRIER

DESIGN-SPEC N2FLOW PURGE-2 PURGESPE STEAM2 W2 WATER

180
**B.3 Overall Flowsheet Balance**

<table>
<thead>
<tr>
<th>Component</th>
<th>IN (kmol/hr)</th>
<th>OUT (kmol/hr)</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CONVENTIONAL COMPONENTS</strong></td>
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</tr>
<tr>
<td>WATER</td>
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<td>14035.1</td>
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<td>AIR</td>
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<td>ETHYL-01</td>
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<td>O-XYL-01</td>
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<td>INDEN-01</td>
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<td>CARBO-01</td>
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<td>CARBO-02</td>
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<td>CARBO-03</td>
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<td>CELLO-01</td>
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<td>NITROGEN</td>
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<td>OXYGEN</td>
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<td>GUAIA-01</td>
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<td>ALUMI-01</td>
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<td>0.460200</td>
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<tr>
<td><strong>TOTAL BALANCE</strong></td>
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<tr>
<td>MCLE (kmol/hr)</td>
<td>28097.5</td>
<td>29209.0</td>
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<tr>
<td>MASS (kg/hr)</td>
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<td>704793.</td>
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<td>-0.255339E+09</td>
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**CO2 EQUIVALENT SUMMARY**

<table>
<thead>
<tr>
<th>Component</th>
<th>CO2E (KG/HR)</th>
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<tbody>
<tr>
<td>FEED STREAMS</td>
<td>0.00000</td>
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<tr>
<td>PRODUCT STREAMS</td>
<td>47604.1</td>
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<tr>
<td>NET STREAMS</td>
<td>47604.1</td>
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<tr>
<td>UTILITIES</td>
<td>0.00000</td>
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<tr>
<td>TOTAL</td>
<td>47604.1</td>
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</table>

---

**ENTHALPY (CAL/SEC) = -0.145287E+11**
B.4 Block Report

BLOCK:  B-1      MODEL: COMPR
-----------------------------
INLET STREAM:                     FLUE
OUTLET STREAM:                    COMGAS
PROPERTY OPTION SET:    SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN              OUT
RELATIVE DIFF.        TOTAL BALANCE
MOLE(KMOL/HR )         13547.8    13547.8
0.00000
MASS(KG/HR )           398486.    398486.
0.00000
ENTHALPY(CAL/SEC )     0.257739E+07    0.898504E+07
-0.713147

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E         27944.6      KG/HR
PRODUCT STREAMS CO2E     27944.6      KG/HR
NET STREAMS CO2E PRODUCTION  0.00000      KG/HR
UTILITIES CO2E PRODUCTION  0.00000      KG/HR
TOTAL CO2E PRODUCTION     0.00000      KG/HR

*** INPUT DATA ***
ISENTROPIC CENTRIFUGAL COMPRESSOR
PRESSURE CHANGE BAR
1.03421
ISENTROPIC EFFICIENCY
0.88000
MECHANICAL EFFICIENCY
0.90000

*** RESULTS ***
INDICATED HORSEPOWER REQUIREMENT KW
23,608.3
Brake HORSEPOWER REQUIREMENT KW
29,808.4
NET WORK REQUIRED KW
29,808.4
POWER LOSSES KW
2,980.84

ISENTROPIC TEMPERATURE C
906.662
EFFICIENCY (POLYTR/ISENTR) USED
0.88000
OUTLET VAPOR FRACTION
1.00000
HEAD DEVELOPED, M-KGF/KG
21,748.7
MECANICAL EFFICIENCY USED
0.90000
INLET HEAT CAPACITY RATIO
1.32544
INLET VOLUMETRIC FLOW RATE , L/MIN
0.182753+08
OUTLET VOLUMETRIC FLOW RATE, L/MIN
0.108942+08
INLET COMPRESSIBILITY FACTOR
1.00032
OUTLET COMPRESSIBILITY FACTOR
1.00054
AV. ISENT. VOL. EXPONENT
1.31926
AV. ISENT. TEMP EXPONENT
1.31869
AV. ACTUAL VOL. EXPONENT
1.37268
AV. ACTUAL TEMP EXPONENT
1.37209

*** ASSOCIATED UTILITIES ***
UTILITY ID FOR ELECTRICITY U-1
RATE OF CONSUMPTION
2.9808+04 KW
COST
2086.5088 $/HR

BLOCK:  B-2      MODEL: COMPR
-----------------------------
INLET STREAM:                     CATFLUE2
OUTLET STREAM:                    S10
PROPERTY OPTION SET:    SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE
*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
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<tr>
<td>RELATIVE DIFF.</td>
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<tr>
<td>TOTAL BALANCE</td>
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<tr>
<td>MOLE (KMOL/HR)</td>
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<tr>
<td>MASS (KG/HR)</td>
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<td>ENTHALPY (CAL/SEC)</td>
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*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  27944.6 KG/HR
PRODUCT STREAMS CO2E  27944.6 KG/HR
NET STREAMS CO2E PRODUCTION  0.00000 KG/HR
UTILITIES CO2E PRODUCTION  0.00000 KG/HR
TOTAL CO2E PRODUCTION  0.00000 KG/HR

*** INPUT DATA ***

ISENTROPIC CENTRIFUGAL COMPRESSOR
PRESSURE CHANGE  BAR
1.03421
ISENTROPIC EFFICIENCY
0.88000
MECHANICAL EFFICIENCY
0.90000

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT  KW
26,344.8
BRAKE HORSEPOWER REQUIREMENT  KW
29,272.0
NET WORK REQUIRED  KW
2,927.2
ISENTROPIC HORSEPOWER REQUIREMENT  KW
23,183.4
CALCULATED OUTLET PRES  BAR
2.03421
CALCULATED OUTLET TEMP  C
861.456
ISENTROPIC TEMPERATURE  C
842.294
EFFICIENCY (POLYTR/ISENTR) USED
0.88000
OUTLET VAPOR FRACTION
1.00000

HEAD DEVELOPED,  M-KGF/KG
21,357.3
MECHANICAL EFFICIENCY USED
0.90000
INLET HEAT CAPACITY RATIO
1.32544
INLET VOLUMETRIC FLOW RATE , L/MIN
0.182753+08
OUTLET VOLUMETRIC FLOW RATE, L/MIN
0.104770+08
INLET COMPRESSIBILITY FACTOR
1.00032
OUTLET COMPRESSIBILITY FACTOR
1.00056
AV. ISENT. VOL. EXPONENT
1.23845
AV. ISENT. TEMP EXPONENT
1.23790
AV. ACTUAL VOL. EXPONENT
1.27634
AV. ACTUAL TEMP EXPONENT
1.27578

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY              U-1
RATE OF CONSUMPTION                   2.9272+04 KW
COST                                   2049.0406 $/HR

BLOCK:  B-3   MODEL: COMPR
-----------------------------------------------
INLET STREAM: VOLATILE
OUTLET STREAM: S12
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
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<tbody>
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<td>RELATIVE DIFF.</td>
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<tr>
<td>TOTAL BALANCE</td>
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<tr>
<td>MOLE (KMOL/HR)</td>
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<td>MASS (KG/HR)</td>
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<td>39994.3</td>
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<td>-0.572207E-02</td>
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*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  69173.1 KG/HR
PRODUCT STREAMS CO2E  69173.1 KG/HR
NET STREAMS CO2E PRODUCTION  0.00000 KG/HR
**UTILITIES CO2E PRODUCTION** 0.00000 KG/HR
**TOTAL CO2E PRODUCTION** 0.00000 KG/HR

---

**ISENTOPIRIC CENTRIFUGAL COMPRESSOR**

**PRESSURE CHANGE** BAR
3.44738

**ISENTOPIRIC EFFICIENCY**
0.88000

**MECHANICAL EFFICIENCY**
0.90000

---

**RESULTS**

**INDICATED HORSEPOWER REQUIREMENT** KW
322.756

**BRAKE HORSEPOWER REQUIREMENT** KW
358.617

**NET WORK REQUIRED** KW
358.617

**POWER LOSSES** KW
35.8617

**ISENTOPIRIC HORSEPOWER REQUIREMENT** KW
284.025

**CALCULATED OUTLET PRES** BAR
12.4474

**CALCULATED OUTLET TEMP** C
32.6392

**ISENTOPIRIC TEMPERATURE** C
29.5460

**EFFICIENCY (POLYTR/ISENTR) USED**
0.88000

**OUTLET VAPOR FRACTION**
1.00000

**HEAD DEVELOPED, M-KGF/KG**
2,607.00

**MECHANICAL EFFICIENCY USED**
0.90000

**INLET HEAT CAPACITY RATIO**
1.35956

**INLET VOLUMETRIC FLOW RATE , L/MIN**
55,919.8

**OUTLET VOLUMETRIC FLOW RATE, L/MIN**
44,535.7

**INLET COMRESSIBILITY FACTOR**
0.98460

**OUTLET COMRESSIBILITY FACTOR**
0.98650

**AV. ISENT. VOL. EXPONENT**
1.35278

**AV. ACTUAL VOL. EXPONENT**
1.42464

**AV. ACTUAL TEMP EXPONENT**
1.41270

---

**ASSOCIATED UTILITIES**

**UTILITY ID FOR ELECTRICITY** U-1
**RATE OF CONSUMPTION** 358.6174 KW
**COST** 25.1032 $/HR

**BLOCK: B-4 MODEL: COMP**

---

**MASS AND ENERGY BALANCE**

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**CO2 EQUIVALENT SUMMARY**

**FEED STREAMS CO2E** 0.00000 KG/HR
**PRODUCT STREAMS CO2E** 0.00000 KG/HR
**NET STREAMS CO2E PRODUCTION** 0.00000 KG/HR
**UTILITIES CO2E PRODUCTION** 0.00000 KG/HR
**TOTAL CO2E PRODUCTION** 0.00000 KG/HR

---

**INPUT DATA**

**ISENTOPIRIC CENTRIFUGAL COMPRESSOR**

**PRESSURE CHANGE** BAR
1.72369

**ISENTOPIRIC EFFICIENCY**
0.88000

**MECHANICAL EFFICIENCY**
0.90000

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**RESULTS**
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<th>Description</th>
<th>Value</th>
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<tbody>
<tr>
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<td>Brake Horsepower Requirement (KW)</td>
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<tr>
<td>Net Work Required (KW)</td>
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<td>Power Losses (KW)</td>
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<td>Indicated Isontric Horsepower Requirement (KW)</td>
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<td>Isontric Temperature (C)</td>
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<td>Outlet Vapor Fraction</td>
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<td>Head Developed (M-Kgf/Kg)</td>
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<td>Mechanical Efficiency Used</td>
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<td>Outlet Compressibility Factor</td>
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<td>Rate of Consumption (KW)</td>
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** Associated Utilities **

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<th>Utility ID for Electricity</th>
<th>Rate of Consumption (KW)</th>
<th>Cost ($/HR)</th>
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<tbody>
<tr>
<td>U-1</td>
<td>1.36610+04</td>
<td>956.3013</td>
</tr>
</tbody>
</table>

** Mass and Energy Balance **

<table>
<thead>
<tr>
<th>Rel Diff.</th>
<th>Total Balance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mole (kmol/hr)</td>
<td>3109.87</td>
</tr>
<tr>
<td>Mass (kg/hr)</td>
<td>159256.</td>
</tr>
<tr>
<td>Enthalpy (cal/sec)</td>
<td>-0.119053E+09</td>
</tr>
</tbody>
</table>

** CO2 Equivalent Summary **

| Feed Streams CO2E | 69273.0 | KG/HR |
| Product Streams CO2E | 69273.0 | KG/HR |
| Utilities CO2E Production | 0.00000 | KG/HR |
| Total CO2E Production | 0.00000 | KG/HR |

** Input Data **

<table>
<thead>
<tr>
<th>Isontric Centrifugal Compressor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure Change (Bar)</td>
</tr>
<tr>
<td>Isontric Efficiency</td>
</tr>
<tr>
<td>Mechanical Efficiency</td>
</tr>
</tbody>
</table>

** Results **

| Indicated Horsepower Requirement (KW) | 3,290.38 |

185
BRAKE HORSEPOWER REQUIREMENT  KW
3,655.98
NET WORK REQUIRED  KW
3,655.98
POWER LOSSES  KW
365.598
ISENTROPIC HORSEPOWER REQUIREMENT  KW
2,895.53
CALCULATED OUTLET PRES  BAR
2.03421
CALCULATED OUTLET TEMP  C
705.240
ISENTROPIC TEMPERATURE  C
699.028
EFFICIENCY (POLYTR/ISENTR) USED
0.88000
OUTLET VAPOR FRACTION
0.74524
HEAD DEVELOPED, M-KGF/KG
17,815.3
MECHANICAL EFFICIENCY USED
0.90000
INLET HEAT CAPACITY RATIO
1.21403
INLET VOLUMETRIC FLOW RATE, L/MIN
2,387,420.
OUTLET VOLUMETRIC FLOW RATE, L/MIN
1,240,100.
INLET COMPRESSIBILITY FACTOR
0.74544
OUTLET COMPRESSIBILITY FACTOR
0.74567
AV. ISENT. VOL. EXPONENT
1.07366
AV. ISENT. TEMP EXPONENT
1.07318
AV. ACTUAL VOL. EXPONENT
1.08411
AV. ACTUAL TEMP EXPONENT
1.08361

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY  U-1
RATE OF CONSUMPTION  3655.9765  KW
COST  255.9184  $/HR

BLOCK: B-7  MODEL: COMPR
-------------------------------
INLET STREAM: DRY-AIR
OUTLET STREAM: S15
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )
0.00000
MASS(KG/HR )
3000.0
ENTHALPY(CAL/SEC )
222188.-788.479

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  KG/HR
PRODUCT STREAMS CO2E  KG/HR
NET STREAMS CO2E PRODUCTION  KG/HR
UTILITIES CO2E PRODUCTION  KG/HR
TOTAL CO2E PRODUCTION  KG/HR

*** INPUT DATA ***

ISENTROPIC CENTRIFUGAL COMPRESSOR
PRESSURE CHANGE  BAR
1.10216
ISENTROPIC EFFICIENCY
0.88000
MECHANICAL EFFICIENCY
0.90000

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT  KW
932.263
BRAKE HORSEPOWER REQUIREMENT  KW
1,035.85
NET WORK REQUIRED  KW
1,035.85
POWER LOSSES  KW
103.585
ISENTROPIC HORSEPOWER REQUIREMENT  KW
820.392
CALCULATED OUTLET PRES  BAR
2.73694
CALCULATED OUTLET TEMP  C
136.357
ISENTROPIC TEMPERATURE  C
123.087
EFFICIENCY (POLYTR/ISENTR) USED
0.88000
OUTLET VAPOR FRACTION
1.00000
HEAD DEVELOPED, M-KGF/KG
10,038.8
MECHANICAL EFFICIENCY USED
0.90000
INLET HEAT CAPACITY RATIO
1.40448
INLET VOLUMETRIC FLOW RATE, L/MIN 422,415.
OUTLET VOLUMETRIC FLOW RATE, L/MIN 215,008.
INLET COMPRESSIBILITY FACTOR
0.99974
OUTLET COMPRESSIBILITY FACTOR
1.00074
AV. ISENT. VOL. EXPONENT
1.40283
AV. ISENT. TEMP EXPONENT
1.40100
AV. ACTUAL VOL. EXPONENT
1.47143
AV. ACTUAL TEMP EXPONENT
1.46924

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY U-1
RATE OF CONSUMPTION 1035.8479 KW
COST 72.5094 $/HR

BLOCK: C-6 MODEL: COMP
-----------------------------
INLET STREAM: VAP-PRO2
OUTLET STREAM: S11
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

IN RELATIVE DIFF. OUT TOTAL BALANCE
MOLE (KMOL/HR ) 1859.58 1859.58
0.00000 MASS (KG/HR ) 52029.3 52029.3
0.00000 ENTHALPY (CAL/SEC ) -0.211054E+08 -0.199462E+08
-0.549245E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 69273.0 KG/HR
PRODUCT STREAMS CO2E 69273.0 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** INPUT DATA ***

ISENTRIC CENTRIFUGAL COMPRESSOR
OUTLET PRESSURE BAR 9.00000
ISENTRIC EFFICIENCY 0.88000
MECHANICAL EFFICIENCY 0.90000

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT KW 4,853.35
BRAKE HORSEPOWER REQUIREMENT KW 5,392.61
NET WORK REQUIRED KW 5,392.61
POWER LOSSES KW 539.261
ISENTRIC HORSEPOWER REQUIREMENT KW 4,270.95
CALCULATED OUTLET TEMP C 326.815
ISENTRIC TEMPERATURE C 299.379
EFFICIENCY (POLYTR/ISENTR) USED 0.88000
OUTLET VAPOR FRACTION 1.00000
HEAD DEVELOPED, M-KGF/KG 30,134.1
MECHANICAL EFFICIENCY USED 0.90000
INLET HEAT CAPACITY RATIO 1.31101
INLET VOLUMETRIC FLOW RATE, L/MIN 895,919.
OUTLET VOLUMETRIC FLOW RATE, L/MIN 171,663.
INLET COMPRESSIBILITY FACTOR 0.99755
OUTLET COMPRESSIBILITY FACTOR 0.99931
AV. ISENT. VOL. EXPONENT 1.32182
AV. ISENT. TEMP EXPONENT 1.32041
*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY                     U-1
RATE OF CONSUMPTION                       4.9520  KW
COST                                      0.3466  $/HR

BLOCK:  C-9      MODEL: COMP

-------------------------------
INLET STREAM:          N2PURGE2
OUTLET STREAM:         S1
PROPERTY OPTION SET:   SRK   SOAVE-REDLICH-KWONG

**  CO2 EQUIVALENT SUMMARY **

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

**  INPUT DATA **

PRES\'S COMPRESSIBLE COMPRESSOR
PRESSURE CHANGE   BAR

2.75790
ISENTROPIC EFFICIENCY
0.88000
MECHANICAL EFFICIENCY
0.90000

**  RESULTS **

INDICATED  HORSEPOWER REQUIREMENT  KW
4.45680
BRAKE  HORSEPOWER REQUIREMENT  KW
4.95200
NET WORK REQUIRED  KW
4.95200

**  ASSOCIATED UTILITIES **

UTILITY ID FOR ELECTRICITY                     U-1
RATE OF CONSUMPTION                       4.9520  KW
COST                                      0.3466  $/HR

BLOCK:  C-9      MODEL: COMP

-------------------------------
INLET STREAM:          N2PURGE2
OUTLET STREAM:         S1
PROPERTY OPTION SET:   SRK   SOAVE-REDLICH-KWONG

**  MASS AND ENERGY BALANCE  ***

<table>
<thead>
<tr>
<th>RELATIVE DIFF.</th>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(KMOL/HR )</td>
<td>3.56971</td>
<td>3.56971</td>
<td></td>
</tr>
<tr>
<td>MASS(KG/HR   )</td>
<td>100.000</td>
<td>100.000</td>
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<tr>
<td>ENTHALPY(CAL/SEC )</td>
<td>-1.49319</td>
<td>1063.00</td>
<td></td>
</tr>
</tbody>
</table>

*  CO2 EQUIVALENT SUMMARY *

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

**  INPUT DATA **

PRES\'S COMPRESSIBLE COMPRESSOR
PRESSURE CHANGE   BAR

2.75790
ISENTROPIC EFFICIENCY
0.88000
MECHANICAL EFFICIENCY
0.90000

**  RESULTS **

INDICATED  HORSEPOWER REQUIREMENT  KW
4.45680
BRAKE  HORSEPOWER REQUIREMENT  KW
4.95200
NET WORK REQUIRED  KW
4.95200

**  ASSOCIATED UTILITIES **

UTILITY ID FOR ELECTRICITY                     U-1
RATE OF CONSUMPTION                       4.9520  KW
COST                                      0.3466  $/HR

BLOCK:  C-9      MODEL: COMP

-------------------------------
INLET STREAM:          N2PURGE2
OUTLET STREAM:         S1
PROPERTY OPTION SET:   SRK   SOAVE-REDLICH-KWONG

**  MASS AND ENERGY BALANCE  ***
**IN** | **OUT**
--- | ---
TOTAL BALANCE | Mole (kmol/hr) | 870.285 | 870.285
 | Mass (kg/hr) | 26246.3 | 26246.3
0.00000 | Enthalpy (cal/SEC) | -0.751104E+07 | -0.744828E+07
-0.835571E-02

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E | 45395.0 | KG/HR
PRODUCT STREAMS CO2E | 45395.0 | KG/HR
NET STREAMS CO2E PRODUCTION | 0.00000 | KG/HR
UTILITIES CO2E PRODUCTION | 0.00000 | KG/HR
TOTAL CO2E PRODUCTION | 0.00000 | KG/HR

*** INPUT DATA ***
ISENTROPIC CENTRIFUGAL COMPRESSOR
PRESSURE CHANGE BAR | 1.72369
ISENTROPIC EFFICIENCY | 0.88000
MECHANICAL EFFICIENCY | 0.90000

*** RESULTS ***
INDICATED HORSEPOWER REQUIREMENT KW | 262.762
BRAKE HORSEPOWER REQUIREMENT KW | 291.958
NET WORK REQUIRED KW | 291.958
POWER LOSSES KW | 29.1958
ISENTROPIC HORSEPOWER REQUIREMENT KW | 231.231
CALCULATED OUTLET PRES BAR | 14.1711
CALCULATED OUTLET TEMP C | 623.212
ISENTROPIC TEMPERATURE C | 620.291
EFFECTIVENESS (POLYTR/ISENTR) USED | 0.88000
OUTLET VAPOR FRACTION | 1.00000
HEAD DEVELOPED, M-KGF/KG | 3,234.14

**MECHANICAL EFFICIENCY USED**
0.90000

**INLET HEAT CAPACITY RATIO**
1.32365

**INLET VOLUMETRIC FLOW RATE, L/MIN**
84,876.4

**OUTLET VOLUMETRIC FLOW RATE, L/MIN**
76,679.5

**INLET COMPRESSIBILITY FACTOR**
1.00466

**OUTLET COMPRESSIBILITY FACTOR**
1.00522

**AV. ISENT. VOL. EXPONENT**
1.23735

**AV. ISENT. TEMP EXPONENT**
1.23064

**AV. ACTUAL VOL. EXPONENT**
1.27699

**AV. ACTUAL TEMP EXPONENT**
1.26997

*** ASSOCIATED UTILITIES ***
UTILITY ID FOR ELECTRICITY | U-1
RATE OF CONSUMPTION | 291.9582 KW
COST | 20.4371 $/HR

**PROPERTY OPTION SET**: SRK, SOAVE-REDLICH-KWONG

**EQUATION OF STATE**

---

**RELATIVE DIFF.**
TOTAL BALANCE
Mole (kmol/hr) | 14425.6 | 14439.9 | 14.3208
 | Mass (kg/hr) | 425562. | 425562.
-0.399188E-08
ENTHALPY (cal/SEC) | -0.403758E+07 | -0.403758E+07
-0.419593E+08

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E | 73380.1 | KG/HR
PRODUCT STREAMS CO2E | 47544.7 | KG/HR
NET STREAMS CO2E PRODUCTION | -25835.4 | KG/HR
**UTILITIES CO2E PRODUCTION**  0.00000  KG/HR
**TOTAL CO2E PRODUCTION**  -25835.4  KG/HR

*** INPUT DATA ***

**STOICHIOMETRY MATRIX:**

**REACTION # 1:**
SUBSTREAM MIXED :
WATER  3.00  BENZE-01  -1.00  CARBO-02  6.00
OXYGEN  -7.50
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 2:**
SUBSTREAM MIXED :
WATER  4.00  TOLUE-01  -1.00  CARBO-02  7.00
OXYGEN  -9.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 3:**
SUBSTREAM MIXED :
WATER  5.00  ETHYL-01  -1.00  CARBO-02  8.00
OXYGEN  -10.5
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 4:**
SUBSTREAM MIXED :
WATER  5.00  M-XYL-01  -1.00  CARBO-02  8.00
OXYGEN  -10.5
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 5:**
SUBSTREAM MIXED :
WATER  5.00  P-XYL-01  -1.00  CARBO-02  8.00
OXYGEN  -10.5
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 6:**
SUBSTREAM MIXED :
WATER  5.00  O-XYL-01  -1.00  CARBO-02  8.00
OXYGEN  -10.5
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 7:**
SUBSTREAM MIXED :
WATER  5.00  STYRE-01  -1.00  CARBO-02  8.00
OXYGEN  -10.0
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 8:**
SUBSTREAM MIXED :
WATER  3.00  PHENO-01  -1.00  CARBO-02  6.00
OXYGEN  -7.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 9:**
SUBSTREAM MIXED :
WATER  4.00  INDEN-01  -1.00  CARBO-02  9.00
OXYGEN  -11.0
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 10:**
SUBSTREAM MIXED :
WATER  4.00  NAPHT-01  -1.00  CARBO-02  10.0
OXYGEN  -12.0
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 11:**
SUBSTREAM MIXED :
WATER  2.00  METHA-01  -1.00  CARBO-02  1.00
OXYGEN  -2.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 12:**
SUBSTREAM MIXED :
WATER  2.00  ETHYL-02  -1.00  CARBO-02  2.00
OXYGEN  -3.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 14:**
SUBSTREAM MIXED :
WATER  3.00  PROPY-01  -1.00  CARBO-02  3.00
OXYGEN  -4.50
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

**REACTION # 15:**
SUBSTREAM MIXED :
WATER  4.00  1-BUT-01  -1.00  CARBO-02  4.00
OXYGEN  -6.00
SUBSTREAM CIPSD : NO PARTICIPATING COMPONENTS

REACTION # 16:
SUBSTREAM MIXED :
WATER  3.00    1:3-B-01 -1.00 CARBO-02  4.00
OXYGEN -5.50
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

REACTION # 17:
SUBSTREAM MIXED :
WATER  3.00    CARBO-02  8.00 BENZO-01 -1.00
OXYGEN -9.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS

REACTION CONVERSION SPECS: NUMBER=   16
REACTION #   1:
SUBSTREAM:MIXED    KEY COMP:BENZE-01 CONV FRAC:  1.000
REACTION #   2:
SUBSTREAM:MIXED    KEY COMP:TOLUE-01 CONV FRAC:  1.000
REACTION #   3:
SUBSTREAM:MIXED    KEY COMP:ETHYL-01 CONV FRAC:  1.000
REACTION #   4:
SUBSTREAM:MIXED    KEY COMP:M-XYL-01 CONV FRAC:  1.000
REACTION #   5:
SUBSTREAM:MIXED    KEY COMP:P-XYL-01 CONV FRAC:  1.000
REACTION #   6:
SUBSTREAM:MIXED    KEY COMP:O-XYL-01 CONV FRAC:  1.000
REACTION #   7:
SUBSTREAM:MIXED    KEY COMP:STYRE-01 CONV FRAC:  1.000
REACTION #   8:
SUBSTREAM:MIXED    KEY COMP:PHENO-01 CONV FRAC:  1.000
REACTION #   9:
SUBSTREAM:MIXED    KEY COMP:INDEN-01 CONV FRAC:  1.000
REACTION #  10:
SUBSTREAM:MIXED    KEY COMP:NAPHT-01 CONV FRAC:  1.000
REACTION #  11:
SUBSTREAM:MIXED    KEY COMP:METHA-01 CONV FRAC:  1.000
REACTION #  12:
SUBSTREAM:MIXED    KEY COMP:ETHYL-02 CONV FRAC:  1.000
REACTION #  14:
SUBSTREAM:MIXED    KEY COMP:PROPY-01 CONV FRAC:  1.000
REACTION #  15:
SUBSTREAM:MIXED    KEY COMP:1-BUT-01 CONV FRAC:  1.000
REACTION #  16:
SUBSTREAM:MIXED    KEY COMP:1:3-B-01 CONV FRAC:  1.000
REACTION #  17:
SUBSTREAM:MIXED    KEY COMP:BENZO-01 CONV FRAC:  1.000

REACTION EXTENTS:

**RESULTS**

OUTLET TEMPERATURE    C  25.00
OUTLET PRESSURE       BAR  1.0132
HEAT DUTY              CAL/SEC 0.33509E+08
VAPOR FRACTION        1.0000

V-L PHASE EQUILIBRIUM :
<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>K(I)</td>
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<td></td>
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<tr>
<td>WATER</td>
<td>0.22761E-01</td>
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<td>0.22761E-01</td>
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<tr>
<td>CARBO-01</td>
<td>0.38337E-01</td>
<td>0.29278E-08</td>
<td>0.38337E-01</td>
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<tr>
<td>CARBO-02</td>
<td>0.74815E-01</td>
<td>0.56877E-05</td>
<td>0.74815E-01</td>
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<tr>
<td>NITROGEN</td>
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<td>0.74144</td>
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<tr>
<td>OXYGEN</td>
<td>0.12264</td>
<td>0.25175E-06</td>
<td>0.12264</td>
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</tbody>
</table>

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY U-2
RATE OF CONSUMPTION 1.4030+05 KW
COST 9820.6549 $/HR

---

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>RELATIVE DIFF.</th>
<th>IN</th>
<th>OUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BALANCE</td>
<td>3109.87</td>
<td>3109.87</td>
</tr>
<tr>
<td>MOLE (KMOL/HR)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MASS (KG/HR)</td>
<td>159256.</td>
<td>159256.</td>
</tr>
<tr>
<td>ENTHALPY (CAL/SEC)</td>
<td>-0.118267E+09</td>
<td>-0.119839E+09</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 69273.0 KG/HR
PRODUCT STREAMS CO2E 69273.0 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

---

*** INPUT DATA ***

CALCULATION METHOD SOLIDS
SEPARATOR CLASSIFICATION CHARACTERISTIC PARTICLE SIZE
VAPOR RECOVERY TO VAPOR OUTLET 1.00000
SOLIDS RECOVERY TO SOLIDS OUTLET 1.00000
SEPARATION SHARPNESS 0.0
FINES OFFSET 0.0
SPECIFIED PRESSURE 1.01325 BAR
SPECIFIED HEAT DUTY 0.0 CAL/SEC
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

VAPOR FRACTION TO VAPOR OUTLET 1.00000
SOLIDS FRACTION TO SOLID OUTLET 1.00000
SOLIDS LOAD OF VAPOR 0.0
VAPOR LOAD OF SOLIDS 0.0

---

*** CO2 EQUIVALENT SUMMARY ***
### Mass and Energy Balance

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE (kmol/hr)</td>
<td>14161.7</td>
</tr>
<tr>
<td>Mass (kg/hr)</td>
<td>49796.0</td>
</tr>
<tr>
<td>Enthalpy (cal/sec)</td>
<td>-0.920363E+08</td>
</tr>
</tbody>
</table>

**Relative Diff.**

**Total Balance**

<table>
<thead>
<tr>
<th>MOLE (kmol/hr)</th>
<th>14161.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass (kg/hr)</td>
<td>49796.0</td>
</tr>
</tbody>
</table>

**CO₂ Equivalents Summary**

**Feed Streams CO₂E** 27944.6 KG/HR

**Product Streams CO₂E** 27944.6 KG/HR

**Net Streams CO₂E Production** 0.00000 KG/HR

**Utilities CO₂E Production** 0.00000 KG/HR

**Total CO₂E Production** 0.00000 KG/HR

### Input Data

**Separator**

**Classification Characteristic**

**Particle Size**

**Vapor Recovery to Vapor Outlet**

**Solids Recovery to Solids Outlet**

**Separation Sharpness**

**Fines Offset**

**Specified Pressure (Bar)**

1.00000

**Specified Heat Duty (cal/sec)**

0.0

**Convergence Tolerance**

0.000100000

### Results

**Vapor Fraction to Vapor Outlet**

1.00000

**Solids Fraction to Solid Outlet**

1.00000

**Solids Load of Vapor**

0.0

**Vapor Load of Solids**

0.0

**Separation Efficiency for Substream CIPSD**

### Equation of State

**Property Option Set:** SRK, SOAVE-REDLICH-KWONG

### Mass and Energy Balance

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE (kmol/hr)</td>
<td>33.3826</td>
</tr>
<tr>
<td>Mass (kg/hr)</td>
<td>3024.22</td>
</tr>
<tr>
<td>Enthalpy (cal/sec)</td>
<td>-5514.26</td>
</tr>
</tbody>
</table>

**Relative Diff.**

**Total Balance**

<table>
<thead>
<tr>
<th>MOLE (kmol/hr)</th>
<th>33.3826</th>
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**CO₂ Equivalents Summary**

**Feed Streams CO₂E** 97.6574 KG/HR

**Product Streams CO₂E** 97.6574 KG/HR

**Net Streams CO₂E Production** 0.00000 KG/HR

**Utilities CO₂E Production** 0.00000 KG/HR

**Total CO₂E Production** 0.00000 KG/HR

### Input Parameters

**Number of Stages**

27

**Algorithm Option**

**Initialization Option**

**Hydraulic Parameter Calculations**

**Inside Loop Convergence Method**

**Design Specification Method**

**Nested**

**Maximum No. of Outside Loop Iterations**

25

**Maximum No. of Inside Loop Iterations**

10

**Maximum Number of Flash Iterations**

30

**Flash Tolerance**

0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE
0.00010000

**** COL-SPECS ****
CONDENSER TEMPERATURE C
30.0000
MASS REFLUX RATIO
0.71390
MASS DISTILLATE TO FEED RATIO
0.77173

**** PROFILES ****
P-SPEC STAGE 1 PRES, BAR
4.76227

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

**** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***
OUTLET STREAMS

COMPONENT:
DIST BTX-MIX HIGHBOIL
WATER .37868E-02 .99621 .17426E-13
BENZ-01 .10110E-02 .99899 .19822E-09
TOLUE-01 .29588E-03 .99970 .71726E-07
ETHYL-01 .96162E-04 .99989 .19822E-09
M-XYL-01 .83776E-04 .99990 .18256E-04
P-XYL-01 .88061E-04 .99990 .15575E-04
O-XYL-01 .67418E-04 .99980 .69091E-03
STYRE-01 .77987E-04 .99923 .69091E-03
PHENO-01 .94480E-05 .76887 .23113
INDEN-01 .41027E-06 .35867E-01 .96413
NAPHT-01 .63153E-11 .20699E-05 1.0000
METHA-01 .66216 .33784 0.0000
ETHYL-02 .28531 .71469 0.0000
PROPY-01 .72100E-01 .92790 0.0000
1-BUT-01 .22527E-01 .97747 0.0000
1:3-B-01 .19509E-01 .98049 0.0000
CARBO-01 .84918 .15082 0.0000
CARBO-02 .25840 .74160 0.0000
BENZO-01 .13669E-04 .69820 .30179
NITROGEN .88444 .11556 0.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE C
30.0000
BOTTOM STAGE TEMPERATURE C
314.136
TOP STAGE LIQUID FLOW KMOL/HR
19.5267
BOTTOM STAGE LIQUID FLOW KMOL/HR
5.65594
TOP STAGE VAPOR FLOW KMOL/HR
0.66237
BOILUP VAPOR FLOW KMOL/HR
82.3731
MOLAR REFLUX RATIO
82.040
MOLAR BOILUP RATIO
14.5640

CONDENSER DUTY (W/O SUBCOOL) CAL/SEC 166,204
REBOILER DUTY CAL/SEC 200,443

**** MAXIMUM FINAL RELATIVE ERRORS ****
DEW POINT 0.39161E-06 STAGE= 15
BUBBLE POINT 0.56763E-06 STAGE= 6
COMPONENT MASS BALANCE 0.32027E-08 STAGE= 15
COMP-CARBO-02 ENERGY BALANCE 0.11490E-05 STAGE= 13

**** PROFILES ****

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

ENDED
### Mass Flow Profiles

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**Stage Flow Rate**

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**Stage Flow Rate**

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01 0.35820E-02 2 0.25624E-06 0.24808E-02 0.67766E-02 0.12886E-01
01 0.38009E-02 11 0.29872E-02 0.18052E-02 0.40660E-02 0.67632E-02
02 0.20774E-02 12 0.66092E-02 0.18099E-02 0.40771E-02 0.67827E-02
02 0.20837E-02 13 0.14271E-01 0.15312E-02 0.39824E-02 0.67998E-02
02 0.20969E-02 14 0.22636E-02 0.20911E-04 0.10122E-03 0.34157E-03
03 0.17372E-03 22 0.63521E-01 0.43266E-19 0.13816E-16 0.50399E-01
14 0.76550E-13 23 0.89757E-01 0.77232E-21 0.40251E-18 0.25068E-02
15 0.56942E-14 24 0.13565 0.22026E-22 0.17129E-19 0.12906E-01
16 0.43357E-15 25 0.21006 0.32374E-23 0.56115E-20 0.73173E-18
18 0.33047E-16 26 0.31823 0.43698E-23 0.52834E-20 0.95351E-18
19 0.19681E-17 27 0.45479 0.0000 0.0000 0.0000
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NITROGEN
1 0.95078E-02 0.21008 0.53057 0.95367E-01
05 0.10401E-02

**STAGE** WATER BENZE-01 TOLUE-01 ETHYL-01

**STAGE** M-XYL-01

1 0.15531 0.41351E-01 0.12093E-01 0.39296E-01
02 0.34234E-02 2 4.9210 2.0237 1.0948 0.64068
0.6128 11 5.8690 2.9078 1.7848 1.1647
1.1315 12 5.8649 2.8979 1.7843 1.1673
1.1343 13 5.9026 2.9098 1.7997 1.1815
1.1487 14 6.9895 3.6659 2.3826 1.6347
1.6009 22 7.7230 4.1541 2.8544 2.0479
2.0179 23 7.7719 4.1740 2.8823 2.0763
2.0465 24 7.8713 4.2386 2.9470 2.1351
2.1059 25 8.0321 4.3588 3.0582 2.2328
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**MOLE-Y-PROFILE**

**K-VALUES**

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*** ASSOCIATED UTILITIES ***

UTILITY USAGE: U-1 (ELECTRICITY)
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CONDENSER 695.8617
48.7103
REBOILER 839.2149
58.7450
-------------------------------
TOTAL: 1535.0766 KW
107.4554 $/HR

BLOCK: DIST2 MODEL: RADFRAC
-------------------------------
INLETS - S19 STAGE 6
OUTLETS - BTX STAGE 1
PHENOL STAGE 15
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN OUT
RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR ) 27.0643 27.0643
0.000000
MASS(KG/HR ) 2309.30 2309.30
-0.13153E-07
ENTHALPY(CAL/SEC ) -18618.3 -19210.1
0.30803E-01

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 57.1600 KG/HR
PRODUCT STREAMS CO2E 57.1600 KG/HR
NET STREAMS CO2E PRODUCTION -0.45577E-05 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION -0.45577E-05 KG/HR

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**NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS

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### ASSOCIATED UTILITIES

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<th>Cost ($/HR)</th>
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### BLOCK: FLASH3 \ MODEL: FLASH3

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<th>Second Liquid Outlet</th>
<th>Property Option Set</th>
<th>Equation of State</th>
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<td>SRK</td>
<td>SOAVE-REDLICH-KWONG</td>
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### INLET STREAM: VAP-PR0

**Relative Diff.**

**Total Balance**

- **Mole (kmol/hr)**: 1859.58
- **Mass (kg/hr)**: 52029.3

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<thead>
<tr>
<th>Component</th>
<th>Mole (kmol/hr)</th>
<th>Enthalpy (cal/°C)</th>
<th>Output</th>
<th>0.200356E+06</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td></td>
<td></td>
<td>0.230218E+08</td>
<td>-0.231015E+08</td>
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</tbody>
</table>

### **CO2 EQUIVALENT SUMMARY**

<table>
<thead>
<tr>
<th>Component</th>
<th>Mole (kmol/hr)</th>
<th>Molar Mass (kg/kmol)</th>
<th>Production CO2E (kg/hr)</th>
<th>Production CO2E (kmole)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td></td>
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<td>69273.0</td>
<td>69273.0</td>
</tr>
</tbody>
</table>

### INPUT DATA

**Three Phase TP FLASH**

- **Specified Temperature (°C)**: 5.00000
- **Specified Pressure (bar)**: 9.00000
- **Maximum No. Iterations**: 30
- **Convergence Tolerance**: 0.0001

**No Key Component is Specified**

**Key Liquid Stream**: AQUEOUS

**Key Stream for Solids**: AQUEOUS

**OBTAINED RESULTS**

<table>
<thead>
<tr>
<th>Component</th>
<th>F(I)</th>
<th>X1(I)</th>
<th>X2(I)</th>
<th>Y(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>0.272E-01</td>
<td>0.805E-03</td>
<td>0.519E-02</td>
<td>0.225</td>
</tr>
<tr>
<td>ベンゼン</td>
<td>0.715E-02</td>
<td>0.200E+05</td>
<td>0.546E-02</td>
<td>0.284</td>
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<tr>
<td>トルエン</td>
<td>0.181E-02</td>
<td>0.931E+06</td>
<td>0.188E-03</td>
<td>0.103E-01</td>
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<tr>
<td>エチルベンサン</td>
<td>0.530E-03</td>
<td>0.393E+08</td>
<td>0.940E-03</td>
<td>0.514E-01</td>
</tr>
<tr>
<td>エチルウレタン</td>
<td>0.451E-03</td>
<td>0.547E+08</td>
<td>0.940E-03</td>
<td>0.514E-01</td>
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<tr>
<td>トルエン</td>
<td>0.481E-03</td>
<td>0.863E+08</td>
<td>0.297E-03</td>
<td>0.163E-01</td>
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<tr>
<td>メタノール</td>
<td>0.352E-03</td>
<td>0.830E+07</td>
<td>0.689E-03</td>
<td>0.377E-01</td>
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<tr>
<td>プロピオン酸</td>
<td>0.432E-03</td>
<td>0.277E+07</td>
<td>0.831E-03</td>
<td>0.458E-01</td>
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<tr>
<td>フェノール</td>
<td>0.402E-04</td>
<td>0.761E-01</td>
<td>0.983E-03</td>
<td>0.547E-01</td>
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<tr>
<td>マレイン酸</td>
<td>0.463E-04</td>
<td>0.953E+06</td>
<td>0.183E-02</td>
<td>0.102</td>
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<tr>
<td>ナフタリン</td>
<td>0.106E-04</td>
<td>0.907E+05</td>
<td>0.776E-01</td>
<td>0.282E-02</td>
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<tr>
<td>メチルベンサン</td>
<td>38.5</td>
<td>0.368E+06</td>
<td>0.289E-01</td>
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<td>プロピオン酸</td>
<td>6.39</td>
<td>0.218E+06</td>
<td>0.773E-02</td>
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<tr>
<td>ナフタリン</td>
<td>1.02</td>
<td>0.602E+06</td>
<td>0.642E-03</td>
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<td>ベンゼン</td>
<td>0.260</td>
<td>0.123E+08</td>
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<td>ベンゼン</td>
<td>0.216</td>
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CARBO-02  0.139  0.407E-01  0.995E-04  0.194
4.77  0.195E+04
BENZO-01  0.249E-03  0.138E-01  0.338E-09  0.112E-05
0.806E-04  0.330E+04
NITROGEN  0.292E-02  0.233E-04  0.101E-08  0.410E-02
176.  0.405E+07

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY                   U-1
RATE OF CONSUMPTION  333.6847 KW
COST  23.3579 $/HR

BLOCK:  HEATER2  MODEL:  HEATER

INLET STREAM: CAT+FLUE
INLET HEAT STREAM: HEAT
OUTLET STREAM: CATFLUE2
PROPERTY OPTION SET: SRK  SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )  14161.7  14161.7
0.00000
MASS(KG/HR )  497960.  497960.  0.00000
ENTHALPY(CAL/SEC )  -0.983286E+08  -0.983286E+08
0.221861E-12

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  27944.6  KG/HR
PRODUCT STREAMS CO2E  27944.6  KG/HR
NET STREAMS CO2E PRODUCTION  0.00000  KG/HR
UTILITIES CO2E PRODUCTION  0.00000  KG/HR
TOTAL CO2E PRODUCTION  0.00000  KG/HR

*** INPUT DATA ***

TWO PHASE PQ FLASH
SPECIFIED PRESSURE  BAR
1.00000
DUTY FROM INLET HEAT STREAM(S)  CAL/SEC
3,805.370.
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE  0.000100000

*** RESULTS ***

OUTLET TEMPERATURE  C
700.00
OUTLET PRESSURE  BAR
1.00000
OUTLET VAPOR FRACTION  1.00000

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY                   U-2
RATE OF CONSUMPTION  1.5932E+04 KW
COST  1115.2640 $/HR

BLOCK:  HEATER3  MODEL:  HEATER

INLET STREAM: GHG
INLET HEAT STREAM: HEAT2
OUTLET STREAM: GHG-2
PROPERTY OPTION SET: SRK  SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY                   U-2
RATE OF CONSUMPTION  1.5932E+04 KW
COST  1115.2640 $/HR

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  47544.7  KG/HR
PRODUCT STREAMS CO2E  47544.7  KG/HR
NET STREAMS CO2E PRODUCTION  0.00000  KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** INPUT DATA ***

TWO PHASE PQ FLASH
SPECIFIED PRESSURE BAR
1.01325
DUTY FROM INLET HEAT STREAM(S) CAL/SEC
0.335089E+08
MAXIMUM NO. ITERATIONS
30
CONVERGENCE TOLERANCE
0.000100000

*** RESULTS ***

OUTLET TEMPERATURE C
1072.4
OUTLET PRESSURE BAR
1.0132
OUTLET VAPOR FRACTION
1.0000

V-L PHASE EQUILIBRIUM :

COMP F(I) X(I) Y(I) K(I)
WATER 0.22761E-01 0.22761E-01 0.22761E-
01 MISSING
CARBO-01 0.38337E-01 0.38337E-01 0.38337E-
01 MISSING
CARBO-02 0.74815E-01 0.74815E-01 0.74815E-
01 MISSING
NITROGEN 0.74144 0.74144 0.74144
MISSING
OXGEN 0.12264 0.12264 0.12264
MISSING

*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY U-2
RATE OF CONSUMPTION 1.4030E+05 KW
COST 9820.6549 $/HR

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED HOT OUTLET TEMP C
SPECIFIED VALUE 80.0000
LMTD CORRECTION FACTOR 1.0000
**PRESSURE SPECIFICATION:**
- **HOT SIDE PRESSURE DROP** | **BAR**
  - 0.0000
- **COLD SIDE PRESSURE DROP** | **BAR**
  - 0.0000

**HEAT TRANSFER COEFFICIENT SPECIFICATION:**
- **HOT LIQUID** |
  - **COLD LIQUID**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT 2-PHASE** |
  - **COLD LIQUID**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT VAPOR** |
  - **COLD LIQUID**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT LIQUID** |
  - **COLD 2-PHASE**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT 2-PHASE** |
  - **COLD 2-PHASE**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT VAPOR** |
  - **COLD VAPOR**
  - **CAL/SEC-SQCM-K**
  - 0.0203
- **HOT LIQUID** |
  - **COLD VAPOR**
  - **CAL/SEC-SQCM-K**
  - 0.0203

*** OVERALL RESULTS ***

**STREAMS:**

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<tr>
<th>VAP-PROD</th>
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<tbody>
<tr>
<td>VAP-PRO2</td>
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<tr>
<td>T= 6.0000D+02</td>
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<tr>
<td>P= 1.0132D+00</td>
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<tr>
<td>V= 1.0000D+00</td>
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<td>STEAM</td>
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<td>T= 4.1167D+02</td>
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<td>P= 1.7900D+02</td>
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<td>P= 1.7900D+02</td>
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**DUTY AND AREA:**

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<thead>
<tr>
<th>CALCULATED HEAT DUTY</th>
<th>CAL/SEC</th>
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<table>
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<tr>
<th>CALCULATED (REQUIRED) AREA</th>
<th>SQM</th>
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<th>ACTUAL EXCHANGER AREA</th>
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<th>PER CENT OVER-DESIGN</th>
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**HEAT TRANSFER COEFFICIENT:**

<table>
<thead>
<tr>
<th>AVERAGE COEFFICIENT (DIRTY)</th>
<th>CAL/SEC-SQCM-K</th>
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<tbody>
<tr>
<td>UA (DIRTY)</td>
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<tr>
<td>0.0203</td>
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<tr>
<td>LOG-MEAN TEMPERATURE DIFFERENCE:</td>
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<tr>
<td>LMTD CORRECTION FACTOR</td>
<td>C</td>
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<td>80.2978</td>
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| NUMBER OF SHELLS IN SERIES | 1 |

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<th>PRESSURE DROP:</th>
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<tbody>
<tr>
<td>HOTSIDE, TOTAL</td>
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<tr>
<td>0.0000</td>
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<td>COLDSIDE, TOTAL</td>
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*** ZONE RESULTS ***

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<tr>
<th>TEMPERATURE LEAVING EACH ZONE:</th>
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<tbody>
<tr>
<td>HOT</td>
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</tr>
<tr>
<td>HOT IN</td>
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<tr>
<td>HOT OUT</td>
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<td>HOT IN</td>
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<td>HOT OUT</td>
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### EQUATION OF STATE

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### PROPERTY OPTION SET:

- SRK
- SOAVE

### PRESSURE DROP:
- 0.0 BAR

### PRESSURE PROFILE:
- CONSTANT2

### ZONE HEAT TRANSFER AND AREA:

<table>
<thead>
<tr>
<th>ZONE</th>
<th>HEAT DUTY</th>
<th>AREA</th>
<th>LMTD</th>
<th>AVERAGE U</th>
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<td>COLD</td>
<td>1</td>
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### HEATX COLD

- PRESSURE PROFILE: CONSTANT2
- PROPERTY OPTION SET: SRK
- EQUATION OF STATE

### HEATX HOT

- PRESSURE PROFILE: CONSTANT2
- PROPERTY OPTION SET: SRK
- EQUATION OF STATE

212
BLOCK: HEATX2  MODEL: HEATX

HOT SIDE:

PROPERTY OPTION SET:  SRK  SOAVE-REDLICH-KWONG

EQUATION OF STATE

COLD SIDE:

PROPERTY OPTION SET:  SRK  SOAVE-REDLICH-KWONG

EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

RELATIVE DIFF.
TOTAL BALANCE
MOLE (KMOL/HR )  4912.54  4912.54
0.00000
MASS (KG/HR )  107029.
0.00000
ENTHALPY (CAL/SEC )  -0.787901E+08
-0.787901E+08
-0.118792E-07

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  69273.0  KG/HR
PRODUCT STREAMS CO2E  69273.0  KG/HR
NET STREAMS CO2E PRODUCTION  0.00000  KG/HR
UTILITIES CO2E PRODUCTION  0.00000  KG/HR
TOTAL CO2E PRODUCTION  0.00000  KG/HR

*** OVERALL RESULTS ***

STREAMS:

---

CONVERGENCE TOLERANCE
0.000100000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT  HEAT EXCHANGER
SPECIFIED HOT OUTLET TEMP
SPECIFIED VALUE  C
5.0000
LMTD CORRECTION FACTOR
1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP  BAR
0.0000
COLD SIDE PRESSURE DROP  BAR
0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:

HOT LIQUID  COLD LIQUID  CAL/SEC-SQCM-
0.0203
HOT 2-PHASE  COLD LIQUID  CAL/SEC-SQCM-
0.0203
HOT VAPOR  COLD LIQUID  CAL/SEC-SQCM-
0.0203
HOT LIQUID  COLD 2-PHASE  CAL/SEC-SQCM-
0.0203
HOT 2-PHASE  COLD 2-PHASE  CAL/SEC-SQCM-
0.0203
HOT VAPOR  COLD 2-PHASE  CAL/SEC-SQCM-
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HOT LIQUID  COLD VAPOR  CAL/SEC-SQCM-
0.0203
HOT 2-PHASE  COLD VAPOR  CAL/SEC-SQCM-
0.0203
HOT VAPOR  COLD VAPOR  CAL/SEC-SQCM-
0.0203

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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

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<td>P= 9.0000D+00</td>
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<td></td>
<td>V= 1.0000D+00</td>
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<tr>
<td></td>
<td>V= 7.2988D-01</td>
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CW2       | COLD       |<-----
|<----- |
S4
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T= 5.3018D-03 | |
P= 4.1159D+00 | |
P= 4.1159D+00 | |
V= 6.6499D-02 | |
V= 0.0000D+00 | |

DUTY AND AREA:
CALCULATED HEAT DUTY   CAL/SEC
3075623.1730
CALCULATED (REQUIRED) AREA   SQM
1669.4098
ACTUAL EXCHANGER AREA   SQM
1669.4098
PER CENT OVER-DESIGN
0.0000

HEAT TRANSFER COEFFICIENT:
AVERAGE COEFFICIENT (DIRTY)   CAL/SEC-SQCM-K
0.0203
UA (DIRTY)   CAL/SEC-K
338921.9257

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR
1.0000
LMTD (CORRECTED)   C
9.0747
NUMBER OF SHELLS IN SERIES
1

PRESSURE DROP:
HOT SIDE, TOTAL   BAR
0.0000
COLD SIDE, TOTAL   BAR
0.0000

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:
HOT

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ZONE HEAT TRANSFER AND AREA:

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<th>AVERAGE U</th>
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HEATX COLD-TQCU HEATX2 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

| ! DUTY ! PRES ! TEMP ! VFRAC ! |
|----------------|----------------|----------------|----------------|----|
| ! 0.0 ! 4.1159 ! 144.6824 ! 6.6499-02 ! |
| ! 1.4646+05 ! 4.1159 ! 144.6824 ! 4.8413-02 ! |
| ! 2.9292+05 ! 4.1159 ! 144.6824 ! 3.0328-02 ! |
| ! 4.3937+05 ! 4.1159 ! 144.6824 ! 1.2243-02 ! |
| ! 5.3852+05 ! 4.1159 ! 144.6824 ! BUB>0.0 ! |

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### EQUATION OF STATE

| 1.0252+06 | 9.0000 | 142.0650 | 0.00  |
| 7.3229+05 | 4.1159 | 133.9256 | 0.00  |
| 8.7875+05 | 4.1159 | 125.7348 | 0.00  |
| 9.7551+05 | 4.1159 | 120.2977 | 0.00  |
| 1.0252+06 | 4.1159 | 117.4979 | 0.00  |
| 1.1717+06 | 4.1159 | 109.2190 | 0.00  |
| 1.3181+06 | 4.1159 | 100.9041 | 0.00  |
| 1.4646+06 | 4.1159 | 92.0646  | 0.00  |
| 1.6110+06 | 4.1159 | 84.1879  | 0.00  |
| 1.7575+06 | 4.1159 | 75.7899  | 0.00  |
| 1.9040+06 | 4.1159 | 67.3772  | 0.00  |
| 2.0504+06 | 4.1159 | 58.9522  | 0.00  |
| 2.1969+06 | 4.1159 | 50.5192  | 0.00  |
| 2.3433+06 | 4.1159 | 42.0826  | 0.00  |
| 2.4898+06 | 4.1159 | 33.6471  | 0.00  |
| 2.6362+06 | 4.1159 | 25.2171  | 0.00  |
| 2.7827+06 | 4.1159 | 16.7972  | 0.00  |
| 2.9292+06 | 4.1159 | 8.3918   | 0.00  |
| 3.0756+06 | 4.1159 | 5.355    | 0.00  |

### PROPERTY OPTION SET:

- **SRK**
- **SOAVE**

### PRESSURE DROP:

**0.0 BAR**

### PRESSURE PROFILE:

**CONSTANT2**

### EQUATION OF STATE

#### HEATX HOT-TQCUR HEATX2 TQCURV INLET

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<th>VFRAC</th>
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### RELATIVE DIFF.

#### *** MASS AND ENERGY BALANCE ***

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#### *** CO2 EQUIVALENT SUMMARY ***

- **FEED STREAMS CO2E:** 97117.7 KG/HR
- **PRODUCT STREAMS CO2E:** 97117.7 KG/HR
- **NET STREAMS CO2E PRODUCTION:** 0.00000 KG/HR
- **UTILITIES CO2E PRODUCTION:** 0.00000 KG/HR
- **TOTAL CO2E PRODUCTION:** 0.00000 KG/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 0.000000000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED COLD OUTLET TEMP
SPECIFIED VALUE C 600.0000
LMTD CORRECTION FACTOR 1.00000
PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP BAR 0.0000
COLD SIDE PRESSURE DROP BAR 0.0000
HEAT TRANSFER COEFFICIENT SPECIFICATION:
HOT LIQUID COLD LIQUID CAL/SEC-SQCM-K 0.0203
HOT 2-PHASE COLD LIQUID CAL/SEC-SQCM-K 0.0203
HOT VAPOR COLD LIQUID CAL/SEC-SQCM-K 0.0203
HOT LIQUID COLD 2-PHASE CAL/SEC-SQCM-K 0.0203
HOT 2-PHASE COLD 2-PHASE CAL/SEC-SQCM-K 0.0203
HOT VAPOR COLD 2-PHASE CAL/SEC-SQCM-K 0.0203
HOT LIQUID COLD VAPOR CAL/SEC-SQCM-K 0.0203
HOT 2-PHASE COLD VAPOR CAL/SEC-SQCM-K 0.0203
HOT VAPOR COLD VAPOR CAL/SEC-SQCM-K 0.0203

*** OVERALL RESULTS ***

STREAMS:

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<tr>
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DUTY AND AREA:
CALCULATED HEAT DUTY CAL/SEC 195421.2342
CALCULATED (REQUIRED) AREA SQM 18.5538
ACTUAL EXCHANGER AREA SQM 18.5538
PER CENT OVER-DESIGN 0.0000

HEAT TRANSFER COEFFICIENT:
AVERAGE COEFFICIENT (DIRTY) CAL/SEC-SQCM-K 0.0203
UA (DIRTY) CAL/SEC-K 3766.7648

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR 1.0000
LMTD (CORRECTED) C 518.8328
NUMBER OF SHELLS IN SERIES 1
PRESSURE DROP:
HOTSIDE, TOTAL BAR 0.0000
COLDSIDE, TOTAL BAR 0.0000
### Zone Results

**TEMPERATURE LEAVING EACH ZONE:**

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<tr>
<th>Zone</th>
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**ZONE HEAT TRANSFER AND AREA:**

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**HEATX COLD-TQCU HEATX3 TQCURV INLET**

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<th>VFRAC</th>
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**PROPERTY OPTION SET:**

- Constant2
- SRK
- SOAVE-REDLICH-KWONG

**EQUATION OF STATE**

<table>
<thead>
<tr>
<th>DUTY</th>
<th>PRES</th>
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<th>VFRAC</th>
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<tbody>
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---

**BLOCK: HEATX4  MODEL: HEATX**

**HOT SIDE:**

- **INLET STREAM:** N2PURGE
- **OUTLET STREAM:** N2PURGE2
- **PROPERTY OPTION SET:** SRK SOAVE-REDLICH-KWONG
- **EQUATION OF STATE:**

  **COLD SIDE:**

- **INLET STREAM:** S13
- **OUTLET STREAM:** NITRO-2
- **PROPERTY OPTION SET:** SRK SOAVE-REDLICH-KWONG
- **EQUATION OF STATE:**

---

***** MASS AND ENERGY BALANCE *****

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<td>-0.120834E+07</td>
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***** CO2 EQUIVALENT SUMMARY *****

- **FEED STREAMS CO2E:** 45395.0 KG/HR
- **PRODUCT STREAMS CO2E:** 45395.0 KG/HR

---

**NET STREAMS CO2E PRODUCTION:** 0.00000 KG/HR

**UTILITIES CO2E PRODUCTION:** 0.00000 KG/HR

**TOTAL CO2E PRODUCTION:** 0.00000 KG/HR

---

**FLASH SPECS FOR HOT SIDE:**

- **TWO PHASE:** FLASH
- **MAXIMUM NO. ITERATIONS:** 30
- **CONVERGENCE TOLERANCE:** 0.000010000

---

**FLASH SPECS FOR COLD SIDE:**

- **TWO PHASE:** FLASH
- **MAXIMUM NO. ITERATIONS:** 30
- **CONVERGENCE TOLERANCE:** 0.000010000

---

**FLOW DIRECTION AND SPECIFICATION:**

- **COUNTERCURRENT HEAT EXCHANGER**
- **SPECIFIED COLD OUTLET TEMP:** 590.0000
- **LMTD CORRECTION FACTOR:** 1.0000

---

**PRESSURE SPECIFICATION:**

- **HOT SIDE PRESSURE DROP:** BAR
  - Value: 0.0000
- **COLD SIDE PRESSURE DROP:** BAR
  - Value: 0.0000

---

**HEAT TRANSFER COEFFICIENT SPECIFICATION:**

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<tr>
<th>HOT LIQUID</th>
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218
*** OVERALL RESULTS ***

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<td>ACTUAL EXCHANGER AREA</td>
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**COLDSIDE, TOTAL**

**BAR**

0.0000

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*** ZONE RESULTS ***

**TEMPERATURE LEAVING EACH ZONE:**

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**ZONE HEAT TRANSFER AND AREA:**

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**HEATX COLD=TCU HEATX4**

**TQCURV INLET**

---

**PRESSURE PROFILE:**

**CONSTANT2**

**PRESSURE DROP:**

**0.0**

**BAR**

**PROPERTY OPTION SET:**

**SRK**

**SOAVE-REDLICH-KWONG**

**EQUATION OF STATE**

---
## Equation of State

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### Property Option Set: SRK SOAVE

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### Relative Diff.

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**HEATX HOT-TQCUR HEATX4 TQCURV INLET**

**HEATX COLD-TQCUR HEATX5 TQCURV OUTLET**

**Total Balance**

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**Enthalpy (CAL/SEC)**

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<tr>
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<td>-0.722609E+07</td>
<td>-0.722609E+07</td>
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</table>

**Outlet Stream:** N2PURGE3

**Inlet Stream:** S15

---

**Block: HEATX5**

**Model: HEATX**

**Hot Side:**

**Inlet Stream:** S1

**Outlet Stream:** N2PURGE3

**Property Option Set:** SRK SOAVE-REDLICH-KWONG

---

**Cold Side:**

**Inlet Stream:** S15

**Outlet Stream:** DRY-AIR2

**Property Option Set:** SRK SOAVE-REDLICH-KWONG

---

***Mass and Energy Balance***

**In:**

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**Out:**

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### CO2 EQUIVALENT SUMMARY

<table>
<thead>
<tr>
<th></th>
<th>HOT STREAMS CO2E</th>
<th>45395.0  KG/HR</th>
<th>PRODUCT STREAMS CO2E</th>
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<th>NET STREAMS CO2E PRODUCTION</th>
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<th>UTILITIES CO2E PRODUCTION</th>
<th>0.00000  KG/HR</th>
<th>TOTAL CO2E PRODUCTION</th>
<th>0.00000  KG/HR</th>
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### INPUT DATA

**FLASH SPECS FOR HOT SIDE:**
- **TWO PHASE FLASH**
- **MAXIMUM NO. ITERATIONS**: 30
- **CONVERGENCE TOLERANCE**: 0.000100000

**FLASH SPECS FOR COLD SIDE:**
- **TWO PHASE FLASH**
- **MAXIMUM NO. ITERATIONS**: 30
- **CONVERGENCE TOLERANCE**: 0.000100000

**FLOW DIRECTION AND SPECIFICATION:**
- **COUNTERCURRENT HEAT EXCHANGER**
- **SPECIFIED COLD OUTLET TEMP**: C
- **SPECIFIED VALUE**: 300.0000

**LMTD CORRECTION FACTOR**: 1.0000

**PRESSURE SPECIFICATION:**
- **HOT SIDE PRESSURE DROP**: BAR 0.0000
- **COLD SIDE PRESSURE DROP**: BAR 0.0000

**HEAT TRANSFER COEFFICIENT SPECIFICATION:**
- **HOT LIQUID COEFFICIENT**: CAL/SEC-SQCM-K 0.0203
- **COLD LIQUID**: CAL/SEC-SQCM-K
- **HOT 2-PHASE**: CAL/SEC-SQCM-K
- **HOT VAPOR**: CAL/SEC-SQCM-K
- **HOT LIQUID**: CAL/SEC-SQCM-K
- **COLD 2-PHASE**: CAL/SEC-SQCM-K
- **COLD VAPOR**: CAL/SEC-SQCM-K

### OVERALL RESULTS

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<tr>
<th>STREAMS</th>
<th>-----------------</th>
<th>-----------------</th>
<th>-----------------</th>
<th>-----------------</th>
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**DUTY AND AREA:**
- **CALCULATED HEAT DUTY**: CAL/SEC 333973.9062
- **CALCULATED (REQUIRED) AREA**: SQM 4.8601
- **ACTUAL EXCHANGER AREA**: SQM 4.8601
- **PER CENT OVER-DESIGN**: 0.0000

**HEAT TRANSFER COEFFICIENT:**
- **AVERAGE COEFFICIENT (DIRTY)**: CAL/SEC-SQCM-K 0.0203
- **UA (DIRTY)**: CAL/SEC-K 986.6892

**LOG-MEAN TEMPERATURE DIFFERENCE:**
- **LMTD CORRECTION FACTOR**: C 1.0000
- **LMTD (CORRECTED)**: C 338.4793
- **NUMBER OF SHELLS IN SERIES**: 1
PRESSURE DROP:
HOTSIDE, TOTAL                 BAR
0.0000
COLDSIDE, TOTAL                BAR
0.0000

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

HOT

<table>
<thead>
<tr>
<th>HOT IN</th>
<th>VAP</th>
<th>HOT OUT</th>
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<tbody>
<tr>
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COLDOUT | VAP | COLDIN |
|<------|-----|-------|
| 300.0 |     | 136.4 |

---

ZONE HEAT TRANSFER AND AREA:

ZONE   HEAT DUTY   AREA   LMTD  AVERAGE U UA
---     ------------  -----   ----   ------
SQCM-K CAL/SEC  SQM   C    CAL/SEC-K
1  333973.906  4.8601  338.4793  0.0203
986.6892

---

HEATX HOT-TQCUR HEATX5 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

---

HEATX COLD-TQCU HEATX5 TQCURV INLET

PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE
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**BLOCK: HEATX7**  **MODEL: HEATX**

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**HOT SIDE:**

- **INLET STREAM:** N2PURGE3
- **OUTLET STREAM:** N2PURGE4
- **PROPERTY OPTION SET:** SRK
- **EQUATION OF STATE:** SOAVE-REDLICH-KWONG

---

**COLD SIDE:**

- **INLET STREAM:** S7
- **OUTLET STREAM:** STEAM2
- **PROPERTY OPTION SET:** SRK
- **EQUATION OF STATE:** SOAVE-REDLICH-KWONG

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**Mass and Energy Balance**

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**Mass (KG/HR):**

| 29446.3 | 29446.3 |

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**Enthalpy (CAL/SEC):**

| -0.111761E+08 | -0.111761E+08 |

---

**CO2 EQUIVALENT SUMMARY**

- **Feed Streams CO2e:** 45395.0 KG/HR
- **Product Streams CO2e:** 45395.0 KG/HR
- **Net Streams CO2e Production:** 0.0000 KG/HR
- **Utilities CO2e Production:** 0.0000 KG/HR
- **Total CO2e Production:** 0.0000 KG/HR

---

**Input Data**

- **Flash Specs for Hot Side:**
  - Two Phase Flash
  - Maximum No. Iterations: 30
  - Convergence Tolerance: 0.000100000
- **Flash Specs for Cold Side:**
  - Two Phase Flash
  - Maximum No. Iterations: 30
  - Convergence Tolerance: 0.000100000
- **Flow Direction and Specification:**
  - Countercurrent Heat Exchanger
  - Specified Cold Outlet Temp: C 480.0000
  - LMTD Correction Factor: 1.0000
- **Pressure Specification:**
  - Hot Side Pressure Drop: BAR 0.0000
  - Cold Side Pressure Drop: BAR 0.0000
- **Heat Transfer Coefficient Specification:**
  - Hot Liquid Cold Liquid: CAL/SEC-SQCM-K 0.0203
  - Hot Two-Phase Cold Liquid: CAL/SEC-SQCM-K 0.0203
  - Hot Vapor Cold Liquid: CAL/SEC-SQCM-K 0.0203
  - Hot Liquid Cold Two-Phase: CAL/SEC-SQCM-K 0.0203
  - Hot Two-Phase Cold Two-Phase: CAL/SEC-SQCM-K 0.0203
HOT VAPOR  COLD 2-PHASE  CAL/SEC-SQCM-K

0.0203

HOT LIQUID  COLD VAPOR  CAL/SEC-SQCM-K

0.0203

HOT 2-PHASE  COLD VAPOR  CAL/SEC-SQCM-K

0.0203

HOT VAPOR  COLD VAPOR  CAL/SEC-SQCM-K

0.0203

*** OVERALL RESULTS ***

STREAMS:

N2PURGE3   HOT
N2PURGE4
T= 4.9058D+02
T= 1.9264D+02
P= 1.4171D+01
V= 1.0000D+00

STEAM2   COLD
S7
T= 4.8000D+02
T= 2.5501D+01
P= 1.7900D+02
V= 1.0000D+00
V= 0.0000D+00

DUTY AND AREA:

CALCULATED HEAT DUTY  CAL/SEC
682762.1980

CALCULATED (REQUIRED) AREA  SQM
59.6625

ACTUAL EXCHANGER AREA  SQM
59.6625

PER CENT OVER-DESIGN
0.0000

HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY)  CAL/SEC-SQCM-K
0.0203

UA (DIRTY)  CAL/SEC-K
12112.6191

LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR

1.0000

LMTD (CORRECTED)  C
56.3678

NUMBER OF SHELLS IN SERIES  1

PRESSURE DROP:

HOTSIDE, TOTAL  BAR
0.0000

COLDSIDE, TOTAL  BAR
0.0000

*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

HOT IN  VAP  VAP  VAP
HOT OUT
| HOT IN  | VAP  | VAP  | VAP
| HOT OUT

COLD IN  VAP  BOIL  LIQ
COLD OUT

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INLET STREAM: S6
OUTLET STREAM: STEAM3
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG

EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

RELATIVE DIFF.
TOTAL BALANCE
IN
MOLE(KMOL/HR ) 14102.9
MASS(KG/HR ) 408486.
ENTHALPY(CAL/SEC ) -0.357519E+07

-0.852602E-06

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 27944.6 KG/HR
PRODUCT STREAMS CO2E 27944.6 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** OVERALL RESULTS ***
STREAMS:

** HEAT TRANSFER COEFFICIENT SPECIFICATION: **
HOT LIQUID COLD LIQUID CAL/SEC-SQCM-K
HOT 2-PHASE COLD LIQUID CAL/SEC-SQCM-K
HOT VAPOR COLD LIQUID CAL/SEC-SQCM-K
HOT LIQUID COLD 2-PHASE CAL/SEC-SQCM-K
HOT 2-PHASE COLD 2-PHASE CAL/SEC-SQCM-K
HOT VAPOR COLD 2-PHASE CAL/SEC-SQCM-K
HOT LIQUID COLD VAPOR CAL/SEC-SQCM-K
HOT 2-PHASE COLD VAPOR CAL/SEC-SQCM-K
HOT VAPOR COLD VAPOR CAL/SEC-SQCM-K

** OVERALL RESULTS **
STREAMS:

** DUTY AND AREA: **
CALCULATED HEAT DUTY CAL/SEC
2645270.9212
CALCULATED (REQUIRED) AREA SQM
35.9517

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** INLET STREAM: S6 **

** OUTLET STREAM: STEAM3 **

** PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG **

** EQUATION OF STATE **

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** RELATIVE DIFF. **

** TOTAL BALANCE **

** IN **
MOLE(KMOL/HR ) 14102.9
MASS(KG/HR ) 408486.
ENTHALPY(CAL/SEC ) -0.357519E+07

-0.852602E-06

** *** CO2 EQUIVALENT SUMMARY *** **

** FEED STREAMS CO2E 27944.6 KG/HR **

** PRODUCT STREAMS CO2E 27944.6 KG/HR **

** NET STREAMS CO2E PRODUCTION 0.00000 KG/HR **

** UTILITIES CO2E PRODUCTION 0.00000 KG/HR **

** TOTAL CO2E PRODUCTION 0.00000 KG/HR **

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

** FLASH SPECS FOR HOT SIDE: **
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

** FLASH SPECS FOR COLD SIDE: **
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

** FLOW DIRECTION AND SPECIFICATION: **
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED COLD OUTLET TEMP C
765.0000
LMTD CORRECTION FACTOR 1.00000

** PRESSURE SPECIFICATION: **
HOT SIDE PRESSURE DROP BAR
0.0000
COLD SIDE PRESSURE DROP BAR
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**HEATX COLD-TQCU HEATX8 TQCURV INLET**

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**PROPERTY OPTION SET:**
- SRK
- SOAVE-REDLICH-KWONG

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**EQUATION OF STATE**

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HEATX HOT-TQCUR HEATX8  TQCURV INLET
PRESSURE PROFILE: CONSTANT2
PRESSURE DROP: 0.0 BAR
PROPERTY OPTION SET: SRK SOAVE-REDLICH-KWONG
EQUATION OF STATE

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**Mass and Energy Balance**

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<tr>
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<th>OUT</th>
<th>RELATIVE DIFF.</th>
<th>TOTAL BALANCE</th>
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<tbody>
<tr>
<td>MOLE(KMOL/HR)</td>
<td>22211.1</td>
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<tr>
<td>MASS(KG/HR)</td>
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</table>

**CO2 Equivalent Summary**

FEED STREAMS CO2E | 47544.7 | KG/HR |
PRODUCT STREAMS CO2E | 47544.7 | KG/HR |
NET STREAMS CO2E PRODUCTION | 0.00000 | KG/HR |
UTILITIES CO2E PRODUCTION | 0.00000 | KG/HR |
TOTAL CO2E PRODUCTION | 0.00000 | KG/HR |

---

**Input Data**

FLASH SPECS FOR HOT SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS | 30 |
CONVERGENCE TOLERANCE | 0.00010000 |

FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS | 30 |
CONVERGENCE TOLERANCE | 0.00010000 |

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER

SPECIFIED COLD OUTLET TEMP
SPECIFIED VALUE: C

540.0000

LMTD CORRECTION FACTOR: 1.0000

PRESSURE SPECIFICATION:
- HOT SIDE PRESSURE DROP: BAR
  0.0000
- COLD SIDE PRESSURE DROP: BAR
  0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
- HOT LIQUID - COLD LIQUID: CAL/SEC-SQCM-K
  0.0203
- HOT 2-PHASE - COLD LIQUID: CAL/SEC-SQCM-K
  0.0203
- HOT VAPOR - COLD LIQUID: CAL/SEC-SQCM-K
  0.0203
- HOT LIQUID - COLD 2-PHASE: CAL/SEC-SQCM-K
  0.0203
- HOT 2-PHASE - COLD 2-PHASE: CAL/SEC-SQCM-K
  0.0203
- HOT VAPOR - COLD 2-PHASE: CAL/SEC-SQCM-K
  0.0203
- HOT LIQUID - COLD VAPOR: CAL/SEC-SQCM-K
  0.0203
- HOT 2-PHASE - COLD VAPOR: CAL/SEC-SQCM-K
  0.0203
- HOT VAPOR - COLD VAPOR: CAL/SEC-SQCM-K
  0.0203

*** OVERALL RESULTS ***

STREAMS:

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*** ZONE RESULTS ***

TEMPERATURE LEAVING EACH ZONE:

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<tr>
<th>ZONE</th>
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<th>VAP</th>
<th>HOT</th>
<th>VAP</th>
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<tr>
<td>HOT IN</td>
<td>VAP</td>
<td>VAP</td>
<td>HOT OUT</td>
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<td>677.5</td>
<td>95.1</td>
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DUTY AND AREA:
- CALCULATED HEAT DUTY: CAL/SEC
  31487780.9618
- CALCULATED (REQUIRED) AREA: SQM
  681.1704
- ACTUAL EXCHANGER AREA: SQM
  681.1704
- PER CENT OVER-DESIGN: 0.0000

HEAT TRANSFER COEFFICIENT:
- AVERAGE COEFFICIENT (DIRTY): CAL/SEC-SQCM-K
  0.0203
- UA (DIRTY): CAL/SEC-K
  138290.5452

LOG-MEAN TEMPERATURE DIFFERENCE:
- LMTD CORRECTION FACTOR: C
  1.0000
- LMTD (CORRECTED): C
  227.6929
- NUMBER OF SHELLS IN SERIES: 1

PRESSURE DROP:
- HOTSIDE, TOTAL: BAR
  0.0000
- COLDSIDE, TOTAL: BAR
  0.0000

---

229
<p>| | | | | |</p>
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**PROPERTY OPTION SET:** SRK, SOAVE

**PRESSURE DROP:** 0.0 BAR

**PRESSURE PROFILE:** CONSTANT2

**EQUATION OF STATE**

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<thead>
<tr>
<th>DUTY</th>
<th>PRES</th>
<th>TEMP</th>
<th>VFRAC</th>
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**HEATX HOT-TQCUR HEATX9 TQCURV INLET**

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**PROPERTY OPTION SET:** SRK, SOAVE-REDLICH-KWONG

**EQUATION OF STATE**

<table>
<thead>
<tr>
<th>DUTY</th>
<th>PRES</th>
<th>TEMP</th>
<th>VFRAC</th>
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<th>Maximum No. Iterations</th>
<th>Convergence Tolerance</th>
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0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

** *** INPUT DATA ***

<table>
<thead>
<tr>
<th>Two Phase Flash</th>
<th>Maximum No. Iterations</th>
<th>Convergence Tolerance</th>
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0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES

** *** INPUT DATA ***

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<th>Maximum No. Iterations</th>
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0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES
### RELATIVE DIFF.

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<th>OUT</th>
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<tr>
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### CO2 EQUIVALENT SUMMARY

| FEED STREAMS CO2E | 23778.1  KG/HR |
| PRODUCT STREAMS CO2E | 23778.1   KG/HR |
| NET STREAMS CO2E PRODUCTION | 0.00000 KG/HR |
| UTILITIES CO2E PRODUCTION | 0.00000 KG/HR |
| TOTAL CO2E PRODUCTION | 0.00000 KG/HR |

### INPUT DATA

- **Two Phase Flash**
- **Maximum No. Iterations**: 30
- **Convergence Tolerance**: 0.000100000
- **Outlet Pressure**: Minimum of Inlet Stream Pressures

### RESULTS

- **Volumetric Flow Rate**: 55.5853 L/MIN

---

### RELATIVE DIFF.

<table>
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<th>OUT</th>
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</thead>
<tbody>
<tr>
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### CO2 EQUIVALENT SUMMARY

| FEED STREAMS CO2E | 0.00000 KG/HR |
| PRODUCT STREAMS CO2E | 0.00000 KG/HR |
| NET STREAMS CO2E PRODUCTION | 0.00000 KG/HR |
| UTILITIES CO2E PRODUCTION | 0.00000 KG/HR |
| TOTAL CO2E PRODUCTION | 0.00000 KG/HR |

### INPUT DATA

- **Outlet Pressure**: 179.000 BAR
- **Pump Efficiency**: 0.88000
- **Driver Efficiency**: 0.90000
- **Flash Specifications**:
  - Liquid Phase Calculation
  - No Flash Performed
  - Maximum Number of Iterations**: 30
  - Convergence Tolerance**: 0.000100000

### RESULTS

- **Volumetric Flow Rate**: 55.5853 L/MIN
PRESSURE CHANGE  BAR
177.987
NPSH AVAILABLE  M-KGF/KG
10.4982
FLUID POWER  KW
16.4891
BRAKE POWER  KW
18.7376
ELECTRICITY  KW
20.8196
PUMP EFFICIENCY USED
0.88800
NET WORK REQUIRED  KW
20.8196
HEAD DEVELOPED  M-KGF/KG
1,891.60

** ASSOCIATED UTILITIES **

UTILITY ID FOR ELECTRICITY                   U-1
RATE OF CONSUMPTION                      20.8196  KW
COST                                      1.4574  S/HR

BLOCK:  P-2      MODEL: PUMP
--------------------------------------
INLET STREAM:          WATER3
OUTLET STREAM:         S6
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

** MASS AND ENERGY BALANCE **

IN              OUT
RELATIVE DIFF.  TOTAL BALANCE
MOLE(KMOL/HR )            555.084         555.084    0.00000
0.000000
MASS(KG/HR )            10000.0         10000.0    0.000000
0.000000
ENTHALPY(CAL/SEC )  -0.106199E+08  -0.106059E+08
-0.131702E-02

** CO2 EQUIVALENT SUMMARY **

FEED STREAMS CO2E
PRODUCT STREAMS CO2E
NET STREAMS CO2E PRODUCTION
UTILITIES CO2E PRODUCTION
TOTAL CO2E PRODUCTION

** INPUT DATA **

OUTLET PRESSURE  BAR
179.000

PUMP EFFICIENCY
0.88800
DRIVER EFFICIENCY
0.90000

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

** RESULTS **

VOLUMETRIC FLOW RATE  L/MIN
173.704
PRESSURE CHANGE  BAR
178.000
NPSH AVAILABLE  M-KGF/KG
10.3574
FLUID POWER  KW
51.5323
BRAKE POWER  KW
58.5594
ELECTRICITY  KW
65.0660
PUMP EFFICIENCY USED
0.88800
NET WORK REQUIRED  KW
65.0660
HEAD DEVELOPED  M-KGF/KG
1,891.74

** ASSOCIATED UTILITIES **

UTILITY ID FOR ELECTRICITY                   U-1
RATE OF CONSUMPTION                      65.0660  KW
COST                                      4.5546  S/HR

BLOCK:  P-3      MODEL: PUMP
--------------------------------------
INLET STREAM:          WATER4
OUTLET STREAM:         S5
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

** MASS AND ENERGY BALANCE **

IN              OUT
RELATIVE DIFF.  TOTAL BALANCE
MOLE(KMOL/HR )            7771.18         7771.18    0.000000
0.000000

233
**MASS (KG/HR )**

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**CO2 EQUIVALENT SUMMARY**

| FEED STREAMS CO2E | 0.000000000 KG/HR |
| PRODUCT STREAMS CO2E | 0.000000000 KG/HR |
| NET STREAMS CO2E PRODUCTION | 0.000000000 KG/HR |
| UTILITIES CO2E PRODUCTION | 0.000000000 KG/HR |
| TOTAL CO2E PRODUCTION | 0.000000000 KG/HR |

**INPUT DATA**

| OUTLET PRESSURE BAR | 179.000 |
| PUMP EFFICIENCY | 0.88000 |
| DRIVER EFFICIENCY | 0.90000 |

**FLASH SPECIFICATIONS:**

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

**RESULTS**

| VOLUMETRIC FLOW RATE L/MIN | 2431.86 |
| PRESSURE CHANGE BAR | 178.000 |
| NPSH AVAILABLE M-KGF/KG | 10.3574 |
| FLUID POWER KW | 721.452 |
| BRAKE POWER KW | 819.831 |
| ELECTRICITY KW | 910.924 |
| PUMP EFFICIENCY USED | 0.88000 |
| NET WORK REQUIRED KW | 910.924 |
| HEAD DEVELOPED M-KGF/KG | 1891.74 |

**CO2 EQUIVALENT SUMMARY**

| FEED STREAMS CO2E | 0.000000000 KG/HR |
| PRODUCT STREAMS CO2E | 0.000000000 KG/HR |
| NET STREAMS CO2E PRODUCTION | 0.000000000 KG/HR |
| UTILITIES CO2E PRODUCTION | 0.000000000 KG/HR |
| TOTAL CO2E PRODUCTION | 0.000000000 KG/HR |

**INPUT DATA**

| OUTLET PRESSURE BAR | 3.10264 |
| PUMP EFFICIENCY | 0.88000 |
| DRIVER EFFICIENCY | 0.90000 |

**FLASH SPECIFICATIONS:**

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

**RESULTS**

| VOLUMETRIC FLOW RATE L/MIN | 310264 |
| PRESSURE CHANGE BAR | 3.10264 |
| NPSH AVAILABLE M-KGF/KG | 10.5195 |
| FLUID POWER KW | 483619 |

**CO2 EQUIVALENT SUMMARY**

| FEED STREAMS CO2E | 0.000000000 KG/HR |
| PRODUCT STREAMS CO2E | 0.000000000 KG/HR |
| NET STREAMS CO2E PRODUCTION | 0.000000000 KG/HR |
| UTILITIES CO2E PRODUCTION | 0.000000000 KG/HR |
| TOTAL CO2E PRODUCTION | 0.000000000 KG/HR |

**INPUT DATA**

| OUTLET PRESSURE BAR | 935.239 |
| PUMP EFFICIENCY | 3.10264 |
| NPSH AVAILABLE M-KGF/KG | 10.5195 |
| FLUID POWER KW | 483619 |
BRAKE POWER KW
5.49567

ELECTRICITY KW
6.10629

PUMP EFFICIENCY USED
0.88000

NET WORK REQUIRED KW
6.10629

HEAD DEVELOPED M-KGF/KG
32.2791

** Associated Utilities **

UTILITY ID FOR ELECTRICITY                  U-1
RATE OF CONSUMPTION                       6.1063  KW
COST                                      0.4274  $/HR

BLOCK: P-5      MODEL: PUMP
-------------------------
INLET STREAM:          WATER
OUTLET STREAM:         S3
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

** Mass and Energy Balance **

RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )            740.316         740.316
0.000000
MASS(KG/HR )              13337.0         13337.0
0.000000
ENTHALPY(CAL/SEC )        -0.141636E+08 -0.141451E+08
-0.130190E-02

** CO2 Equivalent Summary **

FEED STREAMS CO2E         0.000000 KG/HR
PRODUCT STREAMS CO2E     0.000000 KG/HR
NET STREAMS CO2E PRODUCTION 0.000000 KG/HR
UTILITIES CO2E PRODUCTION 0.000000 KG/HR
TOTAL CO2E PRODUCTION     0.000000 KG/HR

** Input Data **

OUTLET PRESSURE BAR
179.000

PUMP EFFICIENCY
0.88000

DRIVER EFFICIENCY
0.90000

Flash Specifications:

** Liquid Phase Calculation **

NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS 30
TOLERANCE 0.000100000

** Results **

VOLUMETRIC FLOW RATE L/MIN
231.660

PRESSURE CHANGE BAR
175.960

NPISH AVAILABLE M-KGF/KG
32.0357

FLUID POWER KW
67.9383

BRAKE POWER KW
77.2026

ELECTRICITY KW
85.7807

PUMP EFFICIENCY USED
0.88000

NET WORK REQUIRED KW
85.7807

HEAD DEVELOPED M-KGF/KG
1,869.99

** Associated Utilities **

UTILITY ID FOR ELECTRICITY                  U-1
RATE OF CONSUMPTION                      85.7807  KW
COST                                      6.0046  $/HR

BLOCK: P-6      MODEL: PUMP
-------------------------
INLET STREAM:          AQUEOUS
OUTLET STREAM:         S16
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

** Mass and Energy Balance **

RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )            500.053         500.053
0.000000
MASS(KG/HR )              9010.81         9010.81
0.000000
ENTHALPY(CAL/SEC )        -0.962377E+07 -0.962365E+07
-0.124571E-04

** CO2 Equivalent Summary **
FEED STREAMS CO2E             2.24857      KG/HR
PRODUCT STREAMS CO2E          2.24857      KG/HR
NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
UTILITIES CO2E PRODUCTION     0.00000      KG/HR
TOTAL CO2E PRODUCTION         0.00000      KG/HR

*** INPUT DATA ***
PRESSURE CHANGE  BAR           1.72369
PUMP EFFICIENCY                0.88000
DRIVER EFFICIENCY              1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION      NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS   30
TOLERANCE                      0.000010000

*** RESULTS ***
VOLUMETRIC FLOW RATE  L/MIN    153.820
PRESSURE CHANGE  BAR           1.72369
NPSH AVAILABLE  M-KGF/KG       0.0
FLUID POWER        KW           0.44190
BRAKE POWER       KW           0.50216
ELECTRICITY       KW           0.50216
PUMP EFFICIENCY USED          0.88000
NET WORK REQUIRED      KW      0.50216
HEAD DEVELOPED  M-KGF/KG      18.0028

*** ASSOCIATED UTILITIES ***
UTILITY ID FOR ELECTRICITY    U-2
RATE OF CONSUMPTION           0.5022  KW
COST                           3.5151-02 $/HR

PROPERTY OPTION SET: SRK     SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN           OUT
MOL(KMOL/HR)  1326.14  1326.14
MASS(KG/HR)   39994.3  39994.3
ENTHALPY(CAL/SEC) -0.114408E+08 -0.114408E+08

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             69173.1      KG/HR
PRODUCT STREAMS CO2E          69173.1      KG/HR
NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
UTILITIES CO2E PRODUCTION     0.00000      KG/HR
TOTAL CO2E PRODUCTION         0.00000      KG/HR

*** INPUT DATA ***
FRACTION OF FLOW                 STRM=N2PURGE  FRAC= 0.65625

*** RESULTS ***
STREAM= N2PURGE        SPLIT=          0.65625     KEY=  0
STREAM= CARRIER2       SPLIT=          0.34375     KEY=  0

BLOCK: RSTOIC  MODEL: RSTOIC
INLET STREAMS: COKECAT2    S8
OUTLET STREAM:  CAT+FLUE
OUTLET HEAT STREAM:    HEAT
PROPERTY OPTION SET: SRK     SOAVE-REDLICH-KWONG
EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN           OUT
MOL(KMOL/HR)  14796.6  14161.7  -634.963
MASS(KG/HR)   497960.  497960.  0.133325E-07
ENTHALPY(CAL/SEC) -0.983286E+08 -0.983286E+08
*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             0.00000      KG/HR
PRODUCT STREAMS CO2E          27944.6      KG/HR
NET STREAMS CO2E PRODUCTION   27944.6      KG/HR
UTILITIES CO2E PRODUCTION     0.00000      KG/HR
TOTAL CO2E PRODUCTION         27944.6      KG/HR

*** INPUT DATA ***
STOICHIOMETRY MATRIX:
REACTION # 1:
SUBSTREAM MIXED :
CARBO-01  1.00  CARBO-03 -1.00  OXYGEN  -0.500
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS
REACTION # 2:
SUBSTREAM MIXED :
CARBO-02  1.00  CARBO-03 -1.00  OXYGEN  -1.00
SUBSTREAM CIPSD :
NO PARTICIPATING COMPONENTS
REACTION CONVERSION SPECS: NUMBER=    2
REACTION # 1:
SUBSTREAM:MIXED  KEY COMP:CARBO-03  CONV FRAC:  0.000
REACTION # 2:
SUBSTREAM:MIXED  KEY COMP:CARBO-03  CONV FRAC:  1.000

VAPOR FRACTION
1.0000

REACTION EXTENTS:

V-L PHASE EQUILIBRIUM :
K(I)        COMP     F(I)           X(I)           Y(I)
01  0.46868E-01  0.88730E-01  0.46868E-01  0.96547E+07  0.16313  0.15904  0.16313
02  0.94296E+07

*** ASSOCIATED UTILITIES ***
UTILITY ID FOR ELECTRICITY                   U-2
RATE OF CONSUMPTION                    1.5932E+04  KW
COST                                    1115.2640  $/HR

BLOCK:  RYIELD MODEL:  RYIELD
-------------------------------
INLET STREAM:          DRY-BIO
OUTLET STREAM:         S-V-PROD
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE
***********************************************************************
********* PROBLEM IN PSD CALCULATION *********
***********************************************************************
**MASS AND ENERGY BALANCE**

<table>
<thead>
<tr>
<th>RELATIVE DIFF.</th>
<th>TOTAL BALANCE</th>
<th>GENERATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE (KMOL/HR)</td>
<td>303.074</td>
<td>2035.86</td>
</tr>
<tr>
<td>MASS (KG/HR)</td>
<td>45816.8</td>
<td>45816.8</td>
</tr>
<tr>
<td>ENTHALPY (CAL/SEC)</td>
<td>-0.142747E+11</td>
<td>-0.140982E+08</td>
</tr>
</tbody>
</table>

**CO2 EQUIVALENT SUMMARY**

| FEED STREAMS CO2E | 0.00000 | KG/HR |
| PRODUCT STREAMS CO2E | 45494.9 | KG/HR |
| TOTAL CO2E PRODUCTION | 45494.9 | KG/HR |

**INPUT DATA**

- TWO PHASE TP FLASH
- SPECIFIED TEMPERATURE C: 600.000
- SPECIFIED PRESSURE BAR: 2.61419
- MAXIMUM NO. ITERATIONS: 30
- CONVERGENCE TOLERANCE: 0.000100

**MOLE-YIELD**

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<tr>
<th>SUBSTREAM MIXED</th>
<th>WATER</th>
<th>BENZE-01</th>
<th>0.581E-02</th>
<th>TOLUE-01</th>
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<tr>
<td>ETHYL-02</td>
<td>0.647E-02</td>
<td>M-XYL-01</td>
<td>0.113E-02</td>
<td>P-XYL-01</td>
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<tr>
<td>O-XYL-01</td>
<td>0.113E-02</td>
<td>STYRE-01</td>
<td>0.830E-03</td>
<td>PHENO-01</td>
</tr>
<tr>
<td>0.671E-01</td>
<td>0.119E-02</td>
<td>NAPHT-01</td>
<td>0.222E-02</td>
<td>METHA-01</td>
</tr>
<tr>
<td>0.534E-03</td>
<td>0.141E-02</td>
<td>CARBO-01</td>
<td>0.361</td>
<td>CARBO-02</td>
</tr>
<tr>
<td>0.111</td>
<td>0.414</td>
<td>BENZO-01</td>
<td>0.302E-03</td>
<td></td>
</tr>
</tbody>
</table>

**INERTS**

- NITROGEN
- OXYGEN
- ALUMI-01

**RESULTS**

- OUTLET TEMPERATURE C: 600.000
*** ASSOCIATED UTILITIES ***

UTILITY ID FOR ELECTRICITY          U-2
RATE OF CONSUMPTION                 5.9706+07  KW
COST                                 4.1794+06   $/HR

BLOCK:  SPLIT1  MODEL:  FSPLIT
---------
INLET STREAM:  COKECAT1
OUTLET STREAMS:  COKECAT2  DEADCAT
PROPERTY OPTION SET:  SRK  SOAVE-REDLICH-KWONG

EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

RELATIVE DIFF.
TOTAL BALANCE
MOLE(KMOL/HR )  1250.29   1250.29
0.181856E-15
MASS(KG/HR )    107226.    107226.
-0.135712E-15
ENTHALPY(CAL/SEC )  -0.101378E+09  -0.101378E+09
-0.146986E-15

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

ISENTROPIC TURBINE
OUTLET PRESSURE  BAR  0.50000
ISENTROPIC EFFICIENCY  0.88000
MECHANICAL EFFICIENCY  0.90000

*** RESULTS ***

INDICATED HORSEPOWER REQUIREMENT  KW  48,385.3
BRAKE HORSEPOWER REQUIREMENT  KW  43,546.8
NET WORK REQUIRED  KW  43,546.8
POWER LOSSES  KW  4,838.53
ISENTROPIC HORSEPOWER REQUIREMENT  KW  54,983.3
CALCULATED OUTLET TEMP  C  83.1974
ISENTROPIC TEMPERATURE  C  83.1974
EFFICIENCY (POLYTR/ISENTR) USED  0.88000
ISENTROPIC OUTLET VAPOR FRACTION  0.86523
HEAD DEVELOPED, M-KGF/KG  -121,200.
MECHANICAL EFFICIENCY USED
0.90000
INLET HEAT CAPACITY RATIO
1.53996
INLET VOLUMETRIC FLOW RATE, L/MIN
51,606.7
INLET COMPRESSIBILITY FACTOR
0.88670
INLET VOLUMETRIC FLOW RATE, L/MIN
7,862,490.
OUTLET VOLUMETRIC FLOW RATE, L/MIN
7,862,490.
OUTLET COMPRESSIBILITY FACTOR
0.86121
AV. ISENT. VOL. EXPONENT
1.18667
AV. ISENT. TEMP EXPONENT
1.16323
AV. ACTUAL VOL. EXPONENT
1.16997
AV. ACTUAL TEMP EXPONENT
1.16323

BLOCK: VALVE    MODEL: VALVE
-----------------------------
INLET STREAM:          BTX-MIX
OUTLET STREAM:         S19
PROPERTY OPTION SET:   SRK       SOAVE-REDLICH-KWONG
EQUATION OF STATE

***  MASS AND ENERGY BALANCE  ***
IN              OUT
RELATIVE DIFF. TOTAL BALANCE
MOLE (KMOL/HR ) 27.0643  27.0643
0.00000
MASS (KG/HR )    2309.30  2309.30
0.00000
ENTHALPY (CAL/SEC) -18618.4 -18618.3
-0.197946E-05

***  CO2 EQUIVALENT SUMMARY  ***
FEED STREAMS CO2E 57.1600 KG/HR
PRODUCT STREAMS CO2E 57.1600 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** RESULTS ***

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

VALVE PRESSURE DROP BAR
0.76228

*** INPUT DATA ***
VALVE OUTLET PRESSURE BAR
4.00000
VALVE FLOW COEF calc. NO
Appendix C: Material Safety Data Sheets

C.1 Benzene [31]

SIGMA-ALDRICH

SAFETY DATA SHEET

Version 5.8
Revision Date 03/03/2015
Print Date 03/03/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Benzene
Product Number : 401165
Brand : Sigma-Aldrich
Index-No. : 601-020-006
CAS-No. : 71-43-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Skraine Drive
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-6002
Fax : +1 800-325-6252

1.4 Emergency telephone number

Emergency Phone #: (914) 770-0655

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquid (Category 2), H225
Skin irritation (Category 2), H315
Eye irritation (Category 3A), H319
Germ cell mutagenicity (Category 1B), H400
Carcinogenicity (Category 1A), H400
Acute aquatic toxicity (Category 2), H401
For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictograms

Signal word : Danger

Hazard statement(s)
H225 : Highly flammable liquid and vapor.
H315 : Causes serious skin irritation.
H319 : Causes serious eye irritation.
H335 : May cause respiratory irritation.
H336 : May cause respiratory irritation.
H360 : May cause a hazard to the reproductive system.
H401 : Toxic to aquatic life.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Form: Liquid
Molecular weight : 78.11 g/mole
CAS-No. : 71-43-2
EC-No. : 200-705-7
Index-No. : 601-020-006
Registration number : 01/219947/08-44-XXXX

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice : Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of danger area.

Precautionary statement(s)
P210 : Keep container tightly closed.
P240 : Wear resistant gloves and away. equipment.
Use explosion-proof electrical ventilating lighting equipment.
P242 : Use only non-sparking tools.
P243 : Take precautionary measures against static discharge.
P244 : Wash skin thoroughly after handling.
P273 : Avoid release to the environment.
P200 : Wear protective gloves / protective clothing / eye protection / face protection.
P201 + P300 : IF SWALLOWED: Immediately call a POISON CENTER or doctor.
P202 : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
P304 + P340 : IF IN CONTACT WITH EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
P308 : IF INHALED: Remove to fresh air. If not breathing, give artificial respiration.
P311 : IF SWALLOWED: Call a POISON CENTER or doctor.
P304 + P353 : IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P313 : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P331 : IF SWALLOWED: Rinse with plenty of water for several minutes;
P335 + P313 : If skin irritation occurs: Get medical advice / attention.
P337 + P313 : If eye irritation persists: Get medical advice / attention.
P338 : Take off contaminated clothing and wash before reuse.
P332 : In case of fire: Use dry powder, dry chemical or alcohol-resistant foam for extinction.
P405 + P402 : Store in a well-ventilated place. Keep cool.
P411 : Store locked up.
P501 : Dispose of contents / container to an approved waste disposal plant.

5. FIRE-FIGHTING MEASURES

6. ACCIDENTAL RELEASE MEASURES

7. HANDLING AND STORAGE

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

9. PHYSICAL AND CHEMICAL PROPERTIES

10. STABILITY AND REACTIVITY

11. TOXICOLOGICAL INFORMATION

12. ECOLOGICAL INFORMATION

13. DISPOSAL CONSIDERATIONS

14. TRANSPORT INFORMATION

15. REGULATORY INFORMATION

16. OTHER INFORMATION

17. CERTIFICATION

18. ADMISSION TO THE MARKET

19. LABELING INSTRUCTIONS

20. DISCLAIMER

21. ADDITIONAL INFORMATION

22. END OF DOCUMENT

Page 2 of 10
If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial ventilation. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labeling (see section 2.2) and in section 11.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.

5. FIREFIGHTING MEASURES
5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Flash back possible over considerable distance. Container explosion may occur under fire conditions.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES
6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Blow off vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE
7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition. Do not smoke. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully revealed and kept upright to prevent leakage.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

5.6.1 Exposure controls/personal protection

Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>71-43-2</td>
<td></td>
<td>TWA</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.6 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>STEL</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks
Leukemia Substances for which there is a Biological Exposure Index or Indices (see BEIH section)
Acute and chronic exposure

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8. EXPOSURE CONTROL/PERSOAL PROTECTION

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
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<tbody>
<tr>
<td>Benzene</td>
<td>71-43-2</td>
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<td>TWA</td>
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<tr>
<td></td>
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<td>0.6 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
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<tr>
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<td></td>
<td>STEL</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
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</table>

Remarks
Leukemia Substances for which there is a Biological Exposure Index or Indices (see BEIH section)
Acute and chronic exposure

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<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
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</tbody>
</table>

See Table 2-2 for the limits applicable in the operations or sectors excluded in 1910.1029.

The final benzene standard in 1910.1029 applies to all occupational exposures to benzene except some subgroups of industry where exposures are consistently under the action level (i.e., distribution and use of fuels, sealed containers and pipelines, coke production, oil and gas drilling and production, natural gas processing, and the percentage exclusion for liquid mixtures); for the exempted exposures, the benzene limits in Table 2-2 apply.

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</table>

Potential Occupational Carcinogen
See Appendix A.

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
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<tbody>
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Potential Occupational Carcinogen
See Appendix A.

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
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</tbody>
</table>

Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>71-43-2</td>
<td>5-Phenylacetic acid</td>
<td>0.0001 mg/ml</td>
<td>In urine</td>
<td>ACGIH - Biological Exposure Indices (BE)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Acetic acid</td>
<td>0.00005 mg/ml</td>
<td>In urine</td>
<td>ACGIH - Biological Exposure Indices (BE)</td>
</tr>
</tbody>
</table>

Remarks
End of shift (As soon as possible after exposure ceased)
6.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment
Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves' outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 450 min
Material tested: Vitreofit® (KCL 900 / Alconox 2577860, Size M)

Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 450 min
Material tested: Vitreofit® (KCL 900 / Alconox 2577860, Size M)

Data source: KCL GmbH, D-35124 Hanau, phone +49 (0)6659 87300, e-mail sales@KCL.de, test method: EN474
If inhaled, in contact with, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customer. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals. Flame-resistant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Properly dispose of packaging or spillage of this product. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES
9.1 Information on basic physical and chemical properties
a) Appearance: Form: liquid
   Colour: colourless
b) Odour: No data available
c) Odour Threshold: No data available
d) pH: No data available
e) Melting point/freezing point: Melting point/range: 5.5 °C (41.9 °F) - lit.
f) Initial boiling point and boiling range: 88 °C (186 °F) - lit.
g) Flash point: -11.0 °C (12.2 °F) - closed cup
h) Evaporation rate: No data available
i) Flammability (solid, gas): No data available
j) Upper/lower Flammability or explosive limits: Upper explosion limit: 8 % (v) lower explosion limit: 1.5 % (v)
k) Vapour pressure: 221.3 Pa (105.0 mmHg) at 37.7 °C (91 °F)
   66.5 Pa (74.6 mmHg) at 20.0 °C (68 °F)
l) Vapour density: No data available
m) Relative density: 0.874 g/cm³ at 25 °C (77 °F)
   At 40 %, 0.775 g/cm³
n) Water solubility: No data available
o) Partition coefficient octanol/water: No data available
p) Auto-ignition temperature: 532.0 °C (993.6 °F)
q) Decomposition temperature: No data available
r) Viscosity: No data available
s) Explosive properties: No data available
t) Corrosivity properties: No data available

10. STABILITY AND REACTIVITY
10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Reactions may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials
Acids, Bases, Halogens, Strong oxidising agents, Metallic salts

10.6 Hazardous decomposition products
Other decomposition products: No data available
In the event of fire: see section 5.

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects
Acute toxicity
LD50 Oral - Rat: 2,600 mg/kg
LD50 Inhalation - Rat - females: 4 h - 44,700 mg/m³
LD50 Dermal - Rabbit: 8,280 mg/kg
No data available

Signal Word: risk - hazard - safety
12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish
- LD50 - Oncorhynchus mykiss (rainbow trout) - 5.90 mg/l - 96 h
- LC50 - Pimephales promelas (fathead minnow) - 10.00 - 12.00 mg/l - 96 h

Toxicity to algae
- EC50 - Pseudokirchneriella subcapitata (green algae) - 26.00 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability
- Result - Readily biodegradable

12.3 Bioaccumulative potential

Bioconcentration
- Leuciscus idus (Golden orfe) - 3 d - 0.00 mg/l

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be evaluated in the event of unprofessional handling or disposal. Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Bulk in a chemical tank or equipped with an afterburner and scrubber but enter extra care in ignoring this material is highly flammable. Provide surplus and non-recyclable solutions to a licensed disposal company. Contact a licenced professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.
14. TRANSPORT INFORMATION

DOT (US)
UN number: 1114  Class: 3  Packing group: II
Proper shipping name: Benzene
Reportable Quantity (RQ): 10 lbs
Packing Hazard: No

IMDG
UN number: 1114  Class: 3  Packing group: II
Proper shipping name: BENZENE
EMS-No: P-E-5-5

IATA
UN number: 1114  Class: 3  Packing group: II
Proper shipping name: Benzene

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 303 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>71-43-2</td>
</tr>
</tbody>
</table>

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
Benzene
CAS-No: 71-43-2  Revision Date: 2007-07-01

Pennsylvania Right To Know Components
Benzene
CAS-No: 71-43-2  Revision Date: 2007-07-01

New Jersey Right To Know Components
Benzene
CAS-No: 71-43-2  Revision Date: 2007-07-01

California Prop. 65 Components
This product contains a chemical known to the State of California to cause cancer.
Benzene
CAS-No: 71-43-2  Revision Date: 2009-02-01

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Harmful reaction: Acute aquatic toxicity
Asp. Tox.: Aspiration hazard
Carc.: Carcinogenicity
Eye Irrit.: Eye irritation

Flam. Liq.: Flammable liquids
H226: Highly flammable liquid and vapour.
H304: May be fatal if swallowed and enters airways.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H400: May cause genetic defects.
H330: May cause cancer.
H372: Causes damage to organs through prolonged or repeated exposure.
H401: Toxic to aquatic life.

HIMS Rating
Health hazard: 2
Chronic Health Hazard: 1
Flammability: 3
Physical Hazard: 0

NFPA Rating
Health hazard: 2
Fire hazard: 3
Reactivity Hazard: 0

Further Information
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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a
guide. The information in this document is based on the present state of our knowledge and is applicable to the
product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the
product. Sigma-Aldrich Corporation and its Affiliates shall not be liable for any damage resulting from handling or
from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-558-9586

Version: 5.0 Revision Date: 02/26/2015 Print Date: 02/26/2015
C.2 Benzofuran [32]

<table>
<thead>
<tr>
<th>Hazards not otherwise classified (HNOC) or not covered by GHS - none</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzofuran</td>
<td>Flam. Liq. 3, Genc. 2, Aquatic Acute 2, Aquatic Chronic 2, H228, H301, H412</td>
<td>&lt;= 100%</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed

No data available.
5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

For small (incident) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 12).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - no smoking. Take measures to prevent the build-up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Recommended storage temperature 2 - 8°C

7.3 Specific end uses

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSOAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid

b) Colour yellow

c) Odour No data available

d) Odour threshold No data available

e) pH No data available

f) Melting point/freezing point No data available

G) Initial boiling point and range 173 - 175 °C (345 - 347 °F) - fl.

h) Flash point 56 °C (133 °F) - closed cup

i) Evaporation rate No data available

j) Flammability (solid, gas) No data available

k) Upper/lower flammability or explosive limits No data available

l) Reactivity No data available

m) Relative density 1.072 g/cm³ at 25 °C (77 °F)

n) Water solubility No data available

d) Partition coefficient n-octanol/water No data available

e) Auto-ignition temperature No data available

c) Decomposition temperature No data available

f) Viscosity No data available
s) Explosive properties No data available
1) Oxidizing properties No data available

5.2 Other safety information
No data available

10. STABILITY AND REACTIVITY
10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatibility with materials
Strong oxidizing agents

10.6 Hazardous decomposition products
Other decomposition products - No data available
In the event of fire - see Section 6

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects
Acute toxicity
No data available
Inhalation: No data available
Dermal: No data available
LD50 Intraperitoneal - Mouse - 500 mg/kg
Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available
Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
Mouse: lymphocytes
Mutation in mammalian somatic cells:
Hamster: ovary
Sister chromatid exchange

Mouse: Other mutation test systems

Carcinogenicity
Carcinogenicity - Rat: Oral
Carcinogenicity - Mouse: Oral

This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH,
NTP, or EPA classification.

Limited evidence of carcinogenicity in animal studies

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Benzofuran)
ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a
carcinogen or potential carcinogen by ACGIH.
NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a
known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a
carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available
Specific target organ toxicity - single exposure
No data available
Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

12.1 Toxicity
Toxic to fish: LC50 - Pinnaeus promelas (fathead minnow) - 14 mg/l - 96 h

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.
10. DISPOSAL CONSIDERATIONS

11. Waste treatment methods

Product

Items in a chemical container equipped with an asbestos band and stopper but avoid extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US) UN number: 1993 Class: 3 Packing group: III Proper shipping name: Flammable liquids, n.o.s. (Benzofuran)

IMDG UN number: 1993 Class: 3 Packing group: III EMG No: 147-7-6 Proper shipping name: FLAMMABLE LIQUID, N.O.S. (Benzofuran)

IATA UN number: 1993 Class: 3 Packing group: III Proper shipping name: Flammable liquid, n.o.s. (Benzofuran)

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (Da Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right To Know Act.

Pennsylvania Right To Know Components

Benzofuran CAS-No. 271-82-6 Revision Date

New Jersey Right To Know Components

Benzofuran CAS-No. 271-82-6 Revision Date

California Prop. 65 Components

WARNING: This product contains a chemical known to the State of California to cause cancer.

Benzofuran CAS-No. 271-82-6 Revision Date 2020-09-27

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute Acute aquatic toxicity

Aquatic Chronic Chronic aquatic toxicity

GHS Code

GHS01 GHS02 GHS03 GHS04 GHS05 GHS06 GHS07 GHS08 GHS09 GHS10
C.3 Carbon Dioxide [33]

SIGMA-ALDRICH

SAFETY DATA SHEET

Revision Date 07/02/2014
Print Date 02/26/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product Identifiers

Product name: Carbon dioxide

1.2 Relevance of the substance or mixture and use as well as any advice against

use of the substance or mixture

CAS-No.: 124-38-9

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich

3005 Grapes Street
SAINT LOUIS MO 63103
USA

Telephone: +1 800-528-9302
Fax: +1 800-528-9302

1.4 Emergency telephone number

Emergency Ph. No.: (314) 775-5855

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

GHS Classification: Inert gas under pressure (liquefied gas), H280

Simple Asphyxiant.

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram:

Signal word: Warning

Hazard statement(s):

H280: Contains gas under pressure; may explode if heated. May displace oxygen and cause rapid suffocation.

Precautionary statement(s):

P410 + P403: Protect from sunlight. Store in a well-ventilated place.

2.3 Hazards not otherwise classified (RNNC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula: CO2

Molecular Weight: 44.01 g/mol

CAS-No.: 124-38-9

CO2

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice:

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled:

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact:

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact:

Flush eyes with water as a precaution.

If swallowed:

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.2 Indication of any immediate medical attention and special treatment needed

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media:

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon dioxide

5.3 Advice for firefighters

Wear self-contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Clean up promptly by sweeping or vacuuming.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

For precautions see section 2.2.
7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly sealed in a dry and well-ventilated place.
Contents under pressure. Avoid heating above 50°C

7.3 Specific end uses
Apart from the uses mentioned in section 1.3 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide</td>
<td>1344-28-5</td>
<td>PWA</td>
<td>5,000 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>30,000 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Asphyxia</td>
<td>USA, OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>STEL</td>
<td>USA, OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA</td>
<td>USA, OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove’s outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practice. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Breakthrough time: 480 min
Material tested: Carbowax® (KCL 667 / Aldrich Z077647, Size M)

Splash contact
Material: Chloroprene
Minimum layer thickness: 0.6 mm
Breakthrough time: 30 min
Material tested: Camagren® (KCL 722 / Aldrich Z077403, Size M)

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- Appearance: Form: Liquid gas
- Odour: Not detected
- Odour threshold: Not available
- pH: Neutral
- Melting point: -78.6°C (-109.5°F) - lit.
- Initial boiling point: Not available
- Flash point: Not available
- Evaporation rate: Not available
- Flammability (solid, gas): No data available
- Explosive limits: Not available
- Water solubility: Not available
- Partition coefficient: Not available
- Autoignition temperature: Not available
- Decomposition temperature: Not available
- Viscosity: Not available
- Explosive properties: Not available
- Oxidizing properties: Not available

9.2 Other safety information

Data source: KCL GmbH, D-38124 Eichenzell, phone: +49 (0)6551 83 77 000, e-mail: sales@kcl.de, test method: EN 74

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (U) or type ABEK (EN 14937) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

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Aldrich - 291010
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10. STABILITY AND REACTIVITY

10.1 Reactivity
no data available

10.2 Chemical stability
stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
no data available

10.4 Conditions to avoid
no data available

10.5 Incompatible materials
no data available

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 6

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
no data available

Inhalation: no data available

Dermal: no data available

no data available

Skin corrosion/irritation
no data available

Eye irritation
no data available

Respiratory or skin sensitisation
no data available

Gastrointestinal irritation
no data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogenic by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
no data available

no data available

Specific target organ toxicity - single exposure
no data available

Specific target organ toxicity - repeated exposure
no data available

12. ECOLOGICAL INFORMATION

12.1 Toxicity
no data available

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product:
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging:
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1015 Class: 2.2
Proper shipping name: Carbon dioxide

UN number: 1015 Class: 2.2
Proper shipping name: CARBON DIOXIDE

IMDG
Emergency reference code: 3 C-3
EMG-No: 0-0, 5-4

Proper shipping name: Carbon dioxide

IATA
UN number: 1015 Class: 2.2
Proper shipping name: Carbon dioxide

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 303 Components

AddRef: 266/128
Page 6 of 7

AddRef: 266/128
16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

H350 Contains gases under pressure; may explode if heated.
H250 May displace oxygen and cause rapid suffocation.
Press. Gas Gases under pressure
SA Simple Asphyxiant

HMIS Rating
Health Hazard: 0
Chronic Health Hazard: 0
Flammability: 1
Physical Hazard: 1

NFPA Rating
Health Hazard: 0
Fire Hazard: 0
Reactivity Hazard: 0

Further Information
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Preparation Information
Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-352-9655

Version: 3.7  Revision Date: 07/02/2014  Print Date: 02/29/2015
C.4 Carbon Monoxide [34]

SIGMA-ALDRICH
SAFETY DATA SHEET
Version 3.0
Revision Date: 12/19/2014
Print Date: 02/26/2015

1. PRODUCT AND COMPANY IDENTIFICATION
1.1 Product identifiers
Product name: Carbon monoxide

1.2 Relevant identified uses of the substance or mixture and uses advised against

1.3 Details of the supplier of the safety data sheet
Company: Sigma-Aldrich
3001 Spruce Street
SAINT LOUIS MO 63110
USA
Telephone: +1 800-255-7222
Fax: +1 800-255-7222

1.4 Emergency telephone number
Emergency Phone #: (314) 775-5555

2. HAZARDS IDENTIFICATION
2.1 Classification of the substance or mixture
GHS Classification in accordance with 29 CFR 1910 (OSHA HCS): Flammable gases (Category 1, H220).

2.2 GHS Label elements, including precautionary statements
Signal word: Danger
Hazard statement(s): Extremely flammable gas. Contains gas under pressure: may explode if heated. Toxic if inhaled.
Precautionary statement(s): P201: Observe special instructions before use. P202: Do not handle until all safety precautions have been read.

P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P205: Do not breathe dust/fume/gas/mist/vapours/spray.
P244: Wash skin thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P271: Use only outdoors or in a well-ventilated area.
P280: Use personal protective equipment as required.
P304 + P340 + P311: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician.
P305 + P330 + P331: IF exposed or contaminated: Get medical advice/attention.
P303 + P361 + P330 + P331: Take off protective clothing and wash hands after handling.

3. COMPOSITION/INFORMATION ON INGREDIENTS
3.1 Substances
Formula: CO
Molecular weight: 28.01 g/mol
CAS-No.: 000-001-00-2
EC-No.: 1916-001-00-2

3.2 Hazardous components

Component | Classification | Concentration
--- | --- | ---
Carbon monoxide | Flam. Gases 1, Press. Gases, Imp. Gas: Acute Tox. 2; Repr.1, A: STOT GE 1; H220, H300, H331, H360, H372 | <= 100 %

4. FIRST AID MEASURES
4.1 Description of first aid measures
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
If inhaled: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
In case of skin contact: Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.
In case of eye contact: Flush eyes with water as a precaution.
If swallowed: Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.
5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters;
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Clean up promptly by sweeping or vacuum.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.
Contents under pressure.
Storage class (TRGS 510): Oxides

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon monoxide</td>
<td>028-50-1</td>
<td>TWA 50,000 ppm</td>
<td>USA, Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
<td></td>
</tr>
</tbody>
</table>

Remarks: The value in ppm is approximate

TWA 25 ppm USA, ACGIH Threshold Limit Values (TLV)

Carbon monoxide

Substances for which there is a Biological Exposure Index or Indices (see section 9.2)

<table>
<thead>
<tr>
<th>Biological exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
</tr>
<tr>
<td>Carbon monoxide</td>
</tr>
</tbody>
</table>

2

<table>
<thead>
<tr>
<th>Remarks</th>
<th>End of shift (As soon as possible after exposure occurs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon monoxide</td>
<td>25 ppm</td>
</tr>
</tbody>
</table>

2

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye protection
Face shield and safety glasses. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Protective clothing
Material: Butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested: Bulecet® (KOL 697 / Aldrich: 2877947, Size M)

Splash protection
Material: Chloroprene
Minimum layer thickness: 0.8 mm
Break through time: 30 min
Material tested: Camper® (KOL: 722 / Aldrich: 2877493, Size M)

Data source: KOL GmbH. D-350124 Ettenheim, phone +49 (0)6059-87500. e-mail sales@kol.de. test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE-approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Page 3 of 8
Body Protection
Complete suit protecting against chemicals. Flame-retardant antistatic protective clothing. This type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a half-face respirator with multipurpose combination (US) or type R95 (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties
a) Appearance
   Form: Compressed gas
b) Odour
   No data available
c) Odour Threshold
   No data available
d) pH
   No data available
e) Melting point/freezing point
   Melting point/range: -205 °C (-337 °F) - lit.
f) Initial boiling point and boiling range
   -191.5 °C (-312.7 °F) - lit.
g) Flash point
   No data available
h) Evaporation rate
   No data available
i) Flammability (solid, gas)
   No data available
j) Upper/lower Flammability or explosive limits
   Upper explosion limit: 74 % (V)
   Lower explosion limit: 12.2 % (V)
k) Vapour pressure
   No data available
l) Vapour density
   0.87 - (Air = 1.0)
m) Relative density
   No data available
n) Water solubility
   No data available
o) Partition coefficient n-octanol/water
   No data available
p) Auto-ignition temperature
   No data available
q) Decomposition temperature
   No data available
r) Viscosity
   No data available
s) Explosive properties
   No data available
t) Oxidizing properties
   No data available

9.2 Other safety information
Relative vapour density 0.87 - (Air = 1.0)

10. STABILITY AND REACTIVITY
10.1 Reactivity
   No data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   No data available

10.4 Conditions to avoid
   Heat, flames and sparks.

10.5 Incompatible materials
   Sodium/volatile oxides, Oxidizers, Strong oxidizing agents

10.6 Hazardous decomposition products
   Other decomposition products - No data available
   In the event of fire: See section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects
   Acute toxicity
   LC50: Inhalation - Rat: 4 h - 1807 ppm
   Dermal: No data available
   No data available
   Skin corrosion/irritation
   No data available
   No data available
   Serious eye damage/eye irritation
   No data available
   No data available
   Respiratory or skin sensitization
   No data available
   No data available
  Gemini self-replicating
   No data available
   Carcinogenicity
   IARC:
   No component of this product present at levels greater than or equal to 0.1% is identified as a probable, possible, or confirmed human carcinogen by IARC.
   NTP:
   No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
   OSHA:
   No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
   Reproductive toxicity
   Known human reproductive toxin
   No data available
   Specific target organ toxicity - single exposure
   No data available
   Specific target organ toxicity - repeated exposure
   Inhalation - Causes damage to organs through prolonged or repeated exposure.
   Aspiration hazard
   No data available
   Additional Information
   RTECS: FS050000

Blood disorders
Stomach - Injuries - Based on Human Evidence
12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Disaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
No data available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Run in a chemical incinerator equipped with an afterburner and scrubber but extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1016
Class: 2.3 (2.1)
Proper shipping name: Carbon monoxide, compressed
Reportable Quantity (RQ):
Poison Inhalaion Hazard: Hazard zone D

IMDS
UN number: 1016
Class: 2.3 (2.1)
Proper shipping name: CARBON MONOXIDE, COMPRESSED

IATA
UN number: 1016
Class: 2.3 (2.1)
Proper shipping name: Carbon monoxide, compressed
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard, Sudden Release of Pressure Hazard, Chronic Health Hazard, Rehealth Hazard

Massachusetts Right To Know Components

Carbon monoxide 030-05-0 1993-04-24
Pennsylvania Right To Know Components
Carbon monoxide CAS-No. 036-444-3 Revision Date 1993-04-24

New Jersey Right To Know Components
Carbon monoxide CAS-No. 036-444-3 Revision Date 1993-04-24

California Prop. 65 Components:
WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

Carbon monoxide

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Toxicity
Acute toxicity
Flammable gases
Extremely flammable gas.
Combustible gas
Contains gas under pressure, may explode if heated.
Toxic if ingested.
May damage fertility or the unborn child.
Causes damage to organs through prolonged or repeated exposure if inhaled.
Gas under pressure
Reproductive toxicity
Specific target organ toxicity - repeated exposure

Hazard Rating
Health hazard: 3
Chronic Health Hazard: 4
Physical Hazard: 0

NFPA Rating
Health hazard: 3
Flammability: 4
Reactivity: 0

Further information
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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-0666
Version: 3.6 Revision Date: 12/15/2011 Print Date: 02/26/2015
C.5 Ethylbenzene [35]

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product Identifiers

Product name: Ethylbenzene
Product Number: 35,084-4
Brand: Sigma-Aldrich
Index-No.: 001-023-00-4
CAS-No.: 100-41-4

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich
3000 Spruce Street
SAIN LOUIS MO 63109
USA
Telephone: +1-800-325-6332
Fax: +1-800-325-6332
Emergency telephone number:
Emergency Phone #: (314) 778-0566

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS): Flammable liquid (Category 2), H226; Acute toxicity, inhalation (Category 4), H332; Specific target organ toxicity - repeated exposure (Category 2), H273; Aspiration hazard (Category 1), H304; Chronic aquatic toxicity (Category 5), H412.

2.2 GHS Label elements, including precautionary statements

Signal word: Danger
Hazard statement(s): Highly flammable liquid and vapour. May be fatal if swallowed and enters airways. Harmful if inhaled. May cause damage to organs through prolonged or repeated exposure. Harmful to aquatic life with long-lasting effects.
Precautionary statement(s): Keep away from heat, sparks, open flames, hot surfaces. - No smoking. Keep container tightly closed. Ground or bonding equipment.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

<table>
<thead>
<tr>
<th>Substance</th>
<th>Formula</th>
<th>Molecular weight</th>
<th>CAS-No.</th>
<th>El-No.</th>
<th>Index-No.</th>
<th>Hazardous components</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylbenzene</td>
<td>C8H10</td>
<td>106.17 g/mol</td>
<td>100-41-4</td>
<td>202-26-4</td>
<td>001-023-00-4</td>
<td>Flam., Liq., 2, Acute Tox. 4, STOT RE 2, Asp. Tox. 1, Aquatic Chronic 5, H226, H332, H273, H304, H412</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
If inhaled: If breathed in, move into fresh air. If breathing is stopped, give artificial respiration. Consult a physician.
In case of skin contact: Wash off with soap and plenty of water. Consult a physician.
In case of eye contact: Flush eyes with water as a precaution.
If swallowed: Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon dioxide

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, wash up with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and transfer to a container for disposal according to local/national regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. Keep away from sources of ignition - no smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully removed and kept upright to prevent leakage.

Hydroscopic. Storage class (TRGS 510): Flammable liquids.

7.3 Specific end uses
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control Parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylbenzene</td>
<td>100-41-4</td>
<td>TWA</td>
<td>20.00000 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Remarked: Corrosive impact, kidney damage (nephropathy)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylbenzene</td>
<td>100-41-4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).

Skin protection
Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves' outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 410 min
Material tested: Vistoject® (KCL 600 / Aldrich 267700, Size M)
Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 410 min
Material tested: Vistoject® (KCL 600 / Aldrich 267700, Size M)
data source: KCL GmbH, D-38124 Eichenau, phone +49 (0)9892 97300, e-mail sales@kcl.de, test method: EN 374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body protection
Complete suit protecting against chemicals. Flame resistant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridge as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Form: liquid
   Colour: colourless
b) Odour: No data available
c) Odour threshold: No data available
d) pH: No data available
e) Melting point/freezing point: Melting point range: 45 °C to 139 °C - lit.
f) Initial boiling point and boiling range: 138 °C (277 °F) - lit.
g) Flash point: 15.0 °C (59.0 °F) - closed cup
h) Evaporation rate: No data available
   (i) Flammability (solid, gas): No data available
   (j) Upper/lower flammability or explosive limits:
      Upper explosion limit: 6.7 % (V)
      Lower explosion limit: 1 % (V)
k) Vapour pressure: 13.3 kPa (100 mmHg) at 20.0 °C (68 °F)
l) Vapour density: No data available
m) Relative density: 0.887 g/cm3 at 25 °C (77 °F)
   (n) Water solubility: 0.2 g/l at 25 °C (77 °F) - slightly soluble
   (o) Partition coefficient, n-octanol/water: log Pow: 3.6 at 20 °C (68 °F)
   (p) Autoignition: 432.0 °C (819.0 °F)

9.2 Other safety information
   Temperature:
   (a) Decomposition temperature: No data available
   (b) Viscosity: 0.773 mPa.s at 20 °C (68 °F)
   (c) Explosive properties: No data available
   (d) Oxidising properties: No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
   No data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   Vapours may form explosive mixture with air.

10.4 Conditions to avoid
   Heat, flames and sparks.

10.5 Incompatible materials
   Strong oxidising agents

10.6 Hazardous decomposition products
   Other decomposition products - No data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects
   Acute toxicity
   LD₅₀ Oral - Rat: male and female - 3,600 mg/kg
   Inhalation: No data available
   LD₅₀ Dermal - Rabbit - 15,433 mg/kg
   No data available
   Skin corrosion/irritation
   Skin - Rabbit: Result: Moderate skin irritation - 24 h
   Serious eye damage/eye irritation
   Eyes - Rabbit: Result: Mild eye irritation
   Respiratory or skin sensitisation
   No data available
   Germ cell mutagenicity
   Hamster: ovary
   Result: negative
   Mouse - male and female
   Result: negative
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13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Do not incinerate or incinerate. Prevent the accidental ignition of the material. Report a fire in the material, especially as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Disposal of unopened product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1175 Class: 5
Proper shipping name: Ethylbenzene
Reportable Quantity (RQ): 1000 lbs
Packed class: II

IMDG

UN number: 1175 Class: 3
Proper shipping name: ETHYLBENZENE

IATA

UN number: 1175 Class: 3
Proper shipping name: Ethylbenzene

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313.

Ethylbenzene

CAS-No.: 100-41-4
Revision Date: 2007-07-01

SARA 311/312 Hazards

Fire Hazard, Choking Hazard

Massachusetts Right To Know Components

Ethylbenzene

CAS-No.: 100-41-4
Revision Date: 2007-07-01

Pennsylvania Right To Know Components

Ethylbenzene

CAS-No.: 100-41-4
Revision Date: 2007-07-01

New Jersey Right To Know Components

Ethylbenzene

CAS-No.: 100-41-4
Revision Date: 2007-07-01

California Prop. 65 Components

WARNING! This product contains a chemical known to the State of California to cause cancer. Ethylbenzene

CAS-No.: 100-41-4
Revision Date: 2007-07-01

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.
Acute Toxicity
Acute Chronic
Acute Toxicity
Asphyxiation
Flammable Liquids
H255 Highly flammable liquid and vapour.
H334 May be fatal if inhaled.
H373 May cause damage to organs through prolonged or repeated exposure.
H412 Harmful to aquatic life with long lasting effects.
STOT RE Specific target organ toxicity - repeated exposure

HMSIS Rating
Health hazard: 1
Chronic Health Hazard: 1
Flammability: 3
Physical Hazard: 0
Neurotoxicity: 0

Further Information
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The above information is believed to be correct but does not purport to be an inclusive and shall be used only as a
guide: The information in this document is based on the present state of our knowledge and is applicable to the
product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the
product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling
or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8586

Version: 5.6 Revision Date: 02/06/2015 Print Date: 02/25/2015
C.6 Naphthalene [36]

SIGMA-ALDRICH
SAFETY DATA SHEET

1. PRODUCT AND COMPANY IDENTIFICATION
1.1 Product identifiers
Product name: Naphthalene

2. HAZARDS IDENTIFICATION
2.1 Classification of the substance or mixture
OSHA Classification in accordance with 29 CFR 1910 (OSHA HC)
Flammable solids (Category 2), H229
Acute toxicity, Oral (Category 2), H302
Canicerepositivity (Category 2), H381
Acute aquatic toxicity (Category 1), H410
Chronic aquatic toxicity (Category 1), H410

3. COMPOSITION/INFORMATION ON INGREDIENTS
3.1 Substances
Formula: C10H8
Molecular Weight: 128.17 g/mole
CAS-No.: 51-05-8
EC-No.: 203-046-5
Index-No.: 001-052-00-2

4. FIRST AID MEASURES
4.1 Description of first aid measures
General advice: Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

Skin contact: Wash off with soap and plenty of water. Consult a physician.

Eye contact: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed: Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and in section 11.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.
5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self-contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool exposed containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Sweep up and shovel. Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brooming and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brooming and transfer to a container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Keep away from sources of ignition – No smoking Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameter</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene</td>
<td>81-20-3</td>
<td>IWA 10 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
</tbody>
</table>

Remarks
Eye & Upper Respiratory Tract irritation
Hematologic effects
Eye damage
Not classifiable as a human carcinogen
Danger of cutaneous absorption.

<table>
<thead>
<tr>
<th>STEL</th>
<th>15 ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>USA, ACGIH Threshold Limit Values</td>
<td></td>
</tr>
<tr>
<td>IWA</td>
<td>19 ppm</td>
</tr>
<tr>
<td>50 mg/m³</td>
<td></td>
</tr>
<tr>
<td>USA, OSHA - TABLE 2-1 Limits for Air Contaminants - 1910.1000</td>
<td></td>
</tr>
<tr>
<td>STEL</td>
<td>15 ppm</td>
</tr>
<tr>
<td>75 mg/m³</td>
<td></td>
</tr>
<tr>
<td>USA, OSHA - TABLE 2-1 Limits for Air Contaminants - 1910.1000</td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td>10 ppm</td>
</tr>
<tr>
<td>50 mg/m³</td>
<td></td>
</tr>
<tr>
<td>USA, Occupational Exposure Limits (OSHA) - TABLE 2-1 Limits for Air Contaminants</td>
<td></td>
</tr>
<tr>
<td>The value of (mg/m³) is approximate</td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td>19 ppm</td>
</tr>
<tr>
<td>50 mg/m³</td>
<td></td>
</tr>
<tr>
<td>USA, NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
<tr>
<td>ST</td>
<td>10 ppm</td>
</tr>
<tr>
<td>75 mg/m³</td>
<td></td>
</tr>
<tr>
<td>USA, NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye Protection
Safety glasses with side-shields conforming to EN 106. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin Protection
Handle with gloves (Gloves must be inspected prior to use. Use proper glove removal technique without touching glove’s outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full Contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: DermaFlex® (KCL 740 / Aldrich 2207272, Size M)

Splash Contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: DermaFlex® (KCL 740 / Aldrich 2207272, Size M)

Data source: KCL GmbH, D-59124 Elschenrath, phone 149 0659 8730000, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE-approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals. Flame retardant anti-static protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory Protection
Where risk assessment shows air-purifying respirators are appropriate use a half-face particulate respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a back-up to engineering controls. If the respirator is the
9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Foam solid
b) Odour: no data available
c) Odour Threshold: no data available
d) pH: no data available
e) Melting point/freezing point: Melting point/range: 80 - 82 °C (176 - 180 °F) - lit.
f) Initial boiling point and boiling range: 216 °C (424 °F) - lit.
g) Flash point: 80.0 °C (176.0 °F) - closed cup
h) Boiling range: no data available
i) Flammability (solid, gas): The substance or mixture is a flammable solid with the category 1.
j) Upper/lower flammability or explosive limits: Upper explosion limit: 5.8 % (V)
   Lower explosion limit: 0.0 % (V)
k) Vapour pressure: 1.3 hPa (10.0 mmHg) at 53.0 °C (127.4 °F)
   0.04 hPa (0.3 mmHg) at 25.0 °C (77.0 °F)
l) Vapour density: no data available
m) Relative density: no data available
n) Water solubility: no data available
o) Partition coefficient n-octanol/water: log Pow: 3.30
p) Auto-ignition temperature: 526.0 °C (978.8 °F)
q) Decomposition temperature: no data available
r) Viscosity: no data available
s) Explosive properties: no data available
t) Oxidizing properties: no data available

9.2 Other safety information

Surface tension: 21.8 mN/m at 100.0 °C (212.0 °F)

10. STABILITY AND REACTIVITY

10.1 Reactivity: no data available

10.2 Chemical stability: Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions: no data available

10.4 Conditions to avoid: Heat, flames and sparks. Extreme of temperature and direct sunlight.

10.5 Incompatible materials: Strong oxidizing agents

10.6 Hazardous decomposition products: Other decomposition products: no data available
   In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects:

Acute toxicity:
   LD50 Oral - rat: 400.0 mg/kg
   LC50 Inhalation - rat: 1 h: > 340 mg/m³

Skin corrosion/irritation: no data available

Serious eye damage/eye irritation:
   Eyes - rabbit: no data available
   Result: Mild eye irritation

Respiratory or skin sensitisation: no data available

Genetic mutagenicity: no data available

Carcinogenicity:
   This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.
   Limited evidence of carcinogenicity in animal studies

IARC: Group 2B: Possibly carcinogenic to humans (Naphthalene)
NTP: Reassessibility anticipated to be a human carcinogen (Naphthalene)
OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity:
   no data available

Specific target organ toxicity - single exposure: no data available

Specific target organ toxicity - repeated exposure: no data available

Application hazard: no data available

Additional Information:
   RTECS: QI0520000

Additional information on chemicals and hazardous materials.

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Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer. Naphthalene is retinotoxic and systemic absorption of its vapors above 15 ppm, may result in, cataaracts, optic neuritis, corneal injury, milk irritation, ingestion may produce the following symptoms: hemolytic anemia, hemoglobinemia, nausea, headache, vomiting, gastrointestinal disturbance, convulsions, anemia, kidney injury may occur. Seizures, coma.

Heart:

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish
LC50 - Oncorhynchos mykiss (rainbow trout) - 0.0 - 0.0 mg/l - 96 h
LC50 - Hilsa oblonga (freshwater catfish) - 1.5 - 3.5 mg/l - 96 h
LD50 - other fish - 5.2 - 3.3 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates
EC50 - Daphnia magna (Water flea) - 1.60 - 4.40 mg/l - 48 h

Toxicity to algae
EC50 - No information available. - 33.00 mg/l - 24 h

12.2 Persistence and degradability

Biodegradability
Result: According to the results of tests of biodegradability this product is not readily biodegradable.

12.3 Bioaccumulative potential

Bioaccumulation
Fish
Bioconcentration factor (BCF) - 427 - 1,150

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Very toxic to aquatic life with long lasting effects.

Environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Very toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in lighting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1534 Class: 4.1 Packing group: III

Proper shipping name: Naphthalene, refined
Reportable Quantity (RQ): 100 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1534 Class: 4.1 Packing group: III
EMS-No: F-A, 5-0

Proper shipping name: NAPHTHALENE, REFINED
Marine pollutant: No

IATA
UN number: 1534 Class: 4.1 Packing group: III
Proper shipping name: Naphthalene, refined

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

CAS-No. 91-20-3 Revision Date

SARA 311/312 Hazards
Flammable, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

CAS-No. 91-20-3 Revision Date

Pennsylvania Right To Know Components

CAS-No. 91-20-3 Revision Date

New Jersey Right To Know Components

CAS-No. 91-20-3 Revision Date

California Prop. 65 Components

WARN!!! This product contains a chemical known to the state of California to cause cancer.

CAS-No. 91-20-3 Revision Date

16. OTHER INFORMATION

Full text of H Statements referred to under sections 2 and 3.

Acute Toxicity: Acute toxicity
Acute aquatic toxicity
Chronic aquatic toxicity
Carcinogenicity
Flammable solids
Flammable liquid
Harmful if swallowed
Suspected of causing cancer
Very toxic to aquatic life
Very toxic to aquatic life with long lasting effects.

HHIRI Rating
Health hazard: 2
Chronic Health Hazard: 2
Flammability: 2
Physical Hazard: 2

NFTA Rating
Health hazard: 2
C.7 Phenol [37]
7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameter</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol</td>
<td>108-45-2</td>
<td>TWA</td>
<td>5.000000 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks
- Central Nervous System impairment
- Upper Respiratory Tract irritation
- Lung damage
- Substances for which there is a Biological Exposure Index or Indexes (new BEI section)
- Not classifiable as a human carcinogen
- Danger of spontaneous combustion
- Potential for dental absorption
- C 15.000000 ppm 60.000000 mg/m³ USA. NIOSH Recommended Exposure Limits
- Potential for dental absorption 15 minute cooling value
- TWA 6.000000 ppm 10.000000 mg/m³ USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

Skin designation
- The value in mg/m³ is approximate.

Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenol</td>
<td>108-45-2</td>
<td>Phenol</td>
<td>250mg/g Creatinine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
<td></td>
</tr>
</tbody>
</table>

Remarks
- End of shift (As soon as possible after exposure ceases)

8.2 Exposure controls

Appropriate engineering controls
- Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment
- Eye/face protection
  - Use splash shield and safety glasses
- Respiratory protection
  - Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or BS 1661 (EU).
- Skin protection
  - Use gloves of appropriate materials, thickness and fit.
- Chemical-specific data
  - Material: nitrile rubber
  - Thickness: 0.3 mm
  - Breakthrough time: 480 min
- Material tested to AATCC 65-1991, Size M
- Splatter contact
9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form solid
b) Odour No data available
c) Odour Threshold No data available
d) pH 6.0
e) Melting point/freezing point Melting point/range: 40 - 43 °C (104 - 109 °F) - lit.
f) Initial boiling point and boiling range 182 °C (360 °F) - lit.
g) Flash point 70.0 °C (174.2 °F) - closed cup
h) Evaporation rate No data available
i) Flammability (solid, gas) No data available
j) Upper/lower Upper explosion limit: 0.6 % V
Lower explosion limit: 1.7 % V
k) Vapour pressure 8.5 hPa (4.7 mmHg) at 29.0 °C (84.2 °F)
l) Vapour density No data available
m) Relative density 1.071 g/ml at 20 °C (77 °F)
n) Water solubility 84 g/l at 20 °C (68 °F)

o) Partition coefficient: n-octanol/water Log Pow: 1.40
p) Auto-ignition temperature 715.0 °C (1,310.0 °F)
q) Decomposition temperature No data available
r) Viscosity No data available

9.2 Other safety information

a) Explosive properties No data available
b) Oxidizing properties No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity No data available

10.2 Chemical stability Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions No data available

10.4 Conditions to avoid No data available

10.5 Incompatible materials Strong oxidising agents. Strong bases. Strong acids

10.6 Hazardous decomposition products Other decomposition products - No data available

In the event of fire: see section 4.
12. ECOLOGICAL INFORMATION

12.1 Toxicity
   - Toxicity to fish: LC50 - Leuciscus idus (Golden orfe): 14.00 - 25.00 mg/l - 49 h
   - LC50 - Carassius auratus (goldfish): 26.10 - 86.90 mg/l - 96 h
   - Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna (Water flea): 55 mg/l - 48 h
   - Toxicity to algae: EC50 - Chlorophyllum vulgaris (Fresh water algae): 370.00 mg/l - 96 h

12.2 Persistence and degradability
   - Biodegradation: Result: Readily biodegradable

12.3 Bioaccumulative potential
   - Bioaccumulation: Daphnia pulex (zebra fish) - 5 h
   - 2 mg/l
   - Bioconcentration factor (BCF): 17.5
   - Remarks: Does not bioaccumulate.

12.4 Mobility in soil
   - No data available

12.5 Results of PBT and vPvB assessment
   - PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
   - An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
   - Toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
   - Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
   - Contaminated packaging
     - Dispose of as unusable product.

14. TRANSPORT INFORMATION

D.O.T. (US)
   - UN number: 1671
   - Class: 6.1
   - Packing group: II
   - Proper shipping name: Phenol, solid
   - Reportable Quantity (RQ): 1000 lbs
   - Poison Inhalation Hazard: No

B.N.O.
   - UN number: 1671
   - Class: 6.1
   - Packing group: II
   - Proper shipping name: PHENOL, SOLID
   - EMS-No: F-A, G-A

IATA
   - UN number: 1671
   - Class: 6.1
   - Packing group: II
   - Proper shipping name: Phenol, solid

15. REGULATORY INFORMATION

SARA 302 Components
   - The following components are subject to reporting levels established by SARA Title III, Section 302:
     - Phenol
       - CAS-No.: 108-95-2
       - Revision Date: 2007-07-01

SARA 313 Components
   - The following components are subject to reporting levels established by SARA Title III, Section 313:
     - Phenol
       - CAS-No.: 108-95-2
       - Revision Date: 2007-07-01

SARA 311/312 Hazards
   - Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
   - Phenol
     - CAS-No.: 108-95-2
     - Revision Date: 2007-07-01

Pennsylvania Right To Know Components
   - Phenol
     - CAS-No.: 108-95-2
     - Revision Date: 2007-07-01

New Jersey Right To Know Components
   - Phenol
     - CAS-No.: 108-95-2
     - Revision Date: 2007-07-01

California Prop. 65 Components
   - This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION
   - Full text of H-Statements referred to under sections 2 and 3.
Acute Toxicity

Aquatic Acute
Acute aquatic toxicity

Aquatic Chronic
Chronic aquatic toxicity

Eye Dam.
Serious eye damage

H301
Toxic if swallowed

H311 + H314
Toxic in contact with skin or if inhaled

H311
Toxic in contact with skin.

H314
Causes severe skin burns and eye damage.

H315
Causes serious eye damage.

H311
Toxic if inhaled.

H341
Suspected of causing genetic defects.

H373
May cause damage to organs through prolonged or repeated exposure.

HMIS Rating
Health hazard: 3
Chronic Health Hazard: 1
Flammability: 0
Physical Hazard: 0

NFPA Rating
Health hazard: 3
Fire Hazard: 2
Reactivity Hazard: 0

Further information
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properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling,
or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8656

Version: 5.0 Revision Date: 01/17/2015 Print Date: 02/26/2016
C.8 Styrene

SIGMA-ALDRICH
SAFETY DATA SHEET

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifier
Product name: Styrene

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified uses: Laboratory chemicals. Manufacture of substances

1.3 Details of the supplier of the safety data sheet
Company: Sigma-Aldrich
Address: 3050 Spruce Street
SAINT LOUIS MO 63103 USA
Telephone: +1 800-322-6532
Fax: +1 800-325-5525

1.4 Emergency telephone number
Emergency Phone #: (214) 776-8556

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
GHS Classification: Flammable liquids (Category 3), H225
Acute toxicity, Inhalation (Category 4), H312
Skin Irritation (Category 2A), H315
Eye Irritation (Category 2A), H319
Acute respiratory irritation (Category 2), H401

For the full list of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements
Signal word Warning

Hazard statement(s)
H225 Flammable liquid and vapour.
H312 Causes skin irritation.
H315 Causes serious eye irritation.
H332 Harmful if inhaled.
H401 Toxic to aquatic life.

Precautionary statement(s)
P201 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P220 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.

P241 Use explosion-proof electrical/ventilating/lighting equipment.
P340 Use only non-sparking tools.
P341 Take precautionary measures against static discharge.
P261 Avoid breathing dust/dust mist/vapours.
P262 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P755 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P303 + P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing.
P312 + P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312 + P338 If swallowed: Rinse mouth.
P332 + P335 Specific treatment (see additional information on this label).
P337 + P338 If skin irritation occurs: Get medical advice/attention.
P357 + P338 If eye irritation persists: Get medical advice/attention.
P365 Take off contaminated clothing and wash before reuse.
P403 + P235 Store in a well-ventilated place. Keep cool.
P601 Dispose of contents/container to an approved waste disposal plant.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Phenylacetylene
Vinylbenzene

Formula: C6H5

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of the dangerous area.

Inhalation
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of fire
Use dry chemical, dry chemical or alcohol-resistant foam for extinction.

[Table showing Hazardous components with Classification and Concentration details]
In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most Important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Container explosion may occur under fire conditions. Vapours may form explosive mixture with air.

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully recapped and kept upright to prevent leakage. Light sensitive.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Styrene</td>
<td>100-42-5</td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA: NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>216 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ST</td>
<td>100 ppm</td>
<td>USA: NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>426 mg/m³</td>
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</tr>
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</table>

Remarks: See Table 2.2

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Styrene</td>
<td>100-42-5</td>
<td>TWA</td>
<td>100 ppm</td>
<td>USA: Occupational Exposure Limits (OSHA) - Table 22</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>237.15-100 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>CBEL</td>
<td>200 ppm</td>
<td>USA: Occupational Exposure Limits (OSHA) - Table 22</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td>237.15-100 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Peak</td>
<td>500 ppm</td>
<td>USA: Occupational Exposure Limits (OSHA) - Table 22</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>237.15-100 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA: OSHA - Table 2-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>215 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STELL</td>
<td>100 ppm</td>
<td>USA: OSHA - Table 2-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>435 mg/m³</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA: ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>237.15-100 ppm</td>
<td></td>
</tr>
</tbody>
</table>

Central Nervous System impairment
Upper Respiratory Tract irritation
Peripheral neuropathy
Gastrointestinal irritation

Gastrointestinal irritation
Solutions for which there is a Biological Exposure Index or Indices (see BEII section)
Not classifiable as a human carcinogen

Not classifiable as a human carcinogen

STEL 40 ppm
USA: ACGIH Threshold Limit Values (TLV)

Central Nervous System impairment
Upper Respiratory Tract irritation
Peripheral neuropathy
Solutions for which there is a Biological Exposure Index or Indices (see BEII section)
Not classifiable as a human carcinogen

Solutions for which there is a Biological Exposure Index or Indices (see BEII section)

BIOLOGICAL OCCUPATIONAL EXPOSURE LIMITS

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Styrene</td>
<td>100-42-5</td>
<td>Mandelic acid plus phenylglyoxylic acid</td>
<td>400 mg/l</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEII)</td>
</tr>
</tbody>
</table>

Remarks: End of shift (as soon as possible after exposure ceases)

Systimes: 0.2 mg/l
In venous blood
ACGIH - Biological Exposure Indices (BEII)

Remarks: End of shift (as soon as possible after exposure ceases)

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practices. Wash hands before breaks and at the end of workday.
Personal protective equipment

Eye face protection

Face shield and safety glasses. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Opposite contamination gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 32 min
Material tested: Camflex® (KCL 710 / Abrohol Z577412, Size M)

Splash contact

Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 460 min
Material tested: Vitapur® (KCL 890 / Abrohol Z577008, Size M)

Data source: KCL GmbH, D-39124 Eschenzell, phone +49 (0)6960 67300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN374, contact the supplier of the C8 approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenarios.

Body Protection

Complete suit protecting against chemical, flame resistant and acid resistant protective clothing. The type of protective equipment must be selected according to the concentration and amount of the hazardous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEKN (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a face-supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. Physical and chemical properties

9.1 Information on basic chemical and physical properties

- Appearance: Form liquid, clear
- Colour: colourless
- Odour: no data available
- Odour threshold: no data available
- pH: no data available
- Melting point/ freezing point: Melting point/range: -31 °C (24 °F) - 18 °C
- Initial boiling point and boiling range: 145 - 148 °C (293 - 298 °F) - 180 °C
- Flash point: 32.0 °C (89.6 °F) - closed cup
- Evaporation rate: no data available
- Flammability (solid, gas): no data available

10. Stability and Reactivity

10.1 Reactivity

- no data available

10.2 Chemical stability

Stable under recommended storage conditions. Contains the following stabilisers:
- 4-tert-Butylresorcinol (0.055 %)

10.3 Possibility of hazardous reactions

No dangerous reactions expected. May polymerize on exposure to light. Heat, flames and sparks.

10.4 Conditions to avoid

May polymerize on exposure to light. Heat, flames and sparks.

10.5 Incompatible materials

No information available

10.6 Hazardous decomposition products

Other decomposition products - no data available

11. Toxicological Information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat: 2,850 mg/kg
Remarks: Behavioral Somnolence (general depressed activity). Liver: Other changes.

LC50 Inhalation - rat: 4 h - 12,000 mg/m^3

Dermal: no data available

Skin contact: Irritation

Skin - rabbit

Acute skin irritation

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12. ECOTOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish:
- LC50: Leuciscus idus (Golden orfe) - 17.00 - 60.00 mg/l - 48 h
- NOEC: Pinephles promelas (fathead minnow) - 4 mg/l - 96 h
- LC50: Pinephles promelas (fathead minnow) - 4.09 mg/l - 96 h
- LOEC: Pinephles promelas (fathead minnow) - 7.56 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates:
- EC50: Daphnia magna (Water fleas) - 182.00 mg/l - 24 h

12.2 Persistence and degradability

Biodegradability
- aerobic: Exposure time 28 d
  Result: > 60 % - Readily biodegradable.

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/indet conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Tropic to aquatic life.
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as an unused product.

14. TRANSPORT INFORMATION

DOT (US)
- UN number: 2005
- Class: 3
- Packing group: III
- Proper shipping name: Styrene monomer, stabilized
- Maximum quantity (MQ): 1000 lbs
- Marine pollutant: No
- Poison Inhalation Hazard: No

IMDG
- UN number: 2005
- Class: 3
- Packing group: III
- Proper shipping name: STYRENE MONOMER, STABILIZED
- Marine pollutant: No

IATA
- UN number: 2005
- Class: 3
- Packing group: III
- Proper shipping name: Styrene monomer, stabilized

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

- Styrene
  - CAS-No.: 100-42-5
  - Revision Date: 2007-07-01
- Pennsylvania Right To Know Components
  - Styrene
    - CAS-No.: 100-42-5
    - Revision Date: 2007-07-01
- New Jersey Right To Know Components
  - Styrene
    - CAS-No.: 100-42-5
    - Revision Date: 2007-07-01

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16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.  Acute toxicity
Aquatic Acute  Acute aquatic toxicity
Eye Irrit.  Eye irritation
Flamm. Liq.  Flammable liquids
H225  Flammable liquid and vapour.
H315  Causes skin irritation.
H319  Causes serious eye irritation.
H332  Harmful if inhaled.
H401  Toxic to aquatic life.
Skin Irrit.  Skin irritation

HMS Rating
Health hazard:  2
Chronic Health Hazard:  *
Physical Hazard:  3

NFPA Rating
Health hazard:  2
Fire Hazard:  3
Reactivity Hazard:  0

Further Information
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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a
guide. This information in this document is based on the present state of our knowledge and is applicable to the
product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the
product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling
or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-821-9898

Version: 3.19  Revision Date: 05/12/2014  Print Date: 03/26/2015
C.9 Toluene [39]

SAFETY DATA SHEET

Product name: Toluene

Company: Sigma-Aldrich

Address: 3005 Spruce Street
SAINT LOUIS MO 63103
USA

Emergency Number: (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquid (Category 3), H225
Skin irritation (Category 2), H315
Reproductive toxicity (Category 2), H401
Specific target organ toxicity, single exposure (Category 3), Central nervous system, H306
Specific target organ toxicity, repeated exposure (Category 2), H373
Skin sensitisation (Category 1), H317
Acute aquatic toxicity (Category 2), H410

2.2 Signal word: Danger

2.3 Hazard statements(s):

H225 Highly flammable liquid and vapour.
H315 Causes skin irritation.
H335 May cause respiratory or skin sensitisation.
H301 May cause harm to organs through prolonged or repeated exposure.
H401 Toxic to aquatic life.

Precautionary statement(s):

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P303 Keep container tightly closed.
P304 Use explosion-proof electrical/ventilating/lighting equipment.
P341 Use personal protective equipment/eye protection/face protection.
P370 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P405 Store in a well-ventilated place. Keep container tightly closed.
P403 Store in a well-ventilated place.
P405 Store locked up.
P453 Dispose of contents/container to an approved waste disposal point.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formular: C8H8

Molecular weight: 92.14 g/mol
OSA-No.: 108-88-3
EC-No.: 203-929-0
Index-No.: 681-001-03
Registration number: 01-21184713313-51-XXX

3.2 Hazardous components

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td></td>
<td>100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Expiration: 244011
If inhaled
In case of skin contact
In case of eye contact
If swallowed
Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES
5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES
6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORING
7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment. Keep away from sources of ignition. No smoking. Take measures to prevent the build-up of static electricity charges.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully reclosed and kept upright to prevent leakage.

Store under inert gas.

Storage class (TROGS 510): Flammable liquids

7.3 Specific end uses
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION
8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
<td>TWA 100 ppm</td>
<td>USA, OSHA - TABLE Z-1 Limits for Air Contaminants - 1210.1000</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 150 ppm</td>
<td>USA, OSHA - TABLE Z-1 Limits for Air Contaminants - 1210.1000</td>
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<tr>
<td></td>
<td></td>
<td>TWA 200 ppm</td>
<td>USA, Occupational Exposure Limits (OSHA) - Table Z-2</td>
<td></td>
</tr>
</tbody>
</table>

Remarks
2071-12-82

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>DE</td>
<td>110-82-7</td>
<td>350 ppm</td>
<td>USA, Occupational Exposure Limits (OSHA) - Table Z-2</td>
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<td>USA, Occupational Exposure Limits (OSHA) - Table Z-2</td>
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<td>2071-12-82</td>
<td>USA, Occupational Exposure Limits (OSHA) - Table Z-2</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>TWA 30 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
</tbody>
</table>

Visual impairments
Female reproductive
Pregnancy loss
2014 Adoption
Substances for which there is a Biological Exposure Index or Indices

STV 100 ppm
Toluene

STV 150 ppm

Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
<td>Toluene</td>
<td>0.0200 mg/L</td>
<td>In blood</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

Remarks
Prior to last shift of workweek

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>0.0300 mg/L</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
<tr>
<td></td>
<td>0.0800 mg/L</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
<tr>
<td></td>
<td>0.3000 mg/L</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
Personal protective equipment
Eyewear protection
Face shield and safety glasses. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 400 min
Material tested: Viton® (KCL 890 / Aloechem 2877890, Size M)
Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Viton® (KCL 890 / Aloechem 2877890, Size M)
data source: KCL GmbH, D-38124 Eschborn, phone +49 (0)69 347 80 00, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the C8 approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Body Protection
Complete suit protecting against chemicals. Flame retardant anti-static protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory protection
Where risk assessment shows air purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or GBB (EU).
Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES
9.1 Information on basic physical and chemical properties
a) Appearance
Form: liquid
Colour: colourless
b) Odour
Aromatic

c) Odour Threshold
No data available
d) pH
No data available
e) Melting point/freezing point
Melting point/range: -23 °C (-13 °F)
f) Initial boiling point and boiling range
110 - 111 °C (220 - 222 °F)
g) Flash point
4.0 °C (39.2 °F) - closed cup
h) Evaporation rate
No data available
i) Flammability (pne, gas)
No data available
j) Upper/lower flammability or explosive limits
Upper explosion limit: 7 % (V)
Lower explosion limit: 1.2 % (V)
k) Vapor pressure
29.1 hPa (21.8 mmHg) at 20.0 °C (68.0 °F)
l) Vapor density
No data available
m) Relative density
0.805 g/mL at 25 °C (77 °F)
n) Water solubility
0.5 g/l at 25 °C (77 °F)
o) Partition coefficient n-octanol/water
No data available
p) Auto-ignition temperature
535.0 °C (995.0 °F)
q) Decomposition temperature
No data available
r) Viscosity
No data available
s) Explosive properties
No data available
t) Oxidizing properties
No data available

9.2 Other safety information
No data available

10. STABILITY AND REACTIVITY
10.1 Reactivity
No data available
10.2 Chemical stability
Stable under recommended storage conditions.
10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.
10.4 Conditions to avoid
Heat, flames and sparks.
10.5 Incompatible materials
Strong oxidising agents.
10.6 Hazardous decomposition products
Other decomposition products - No data available
in the event of fire. See section 5.

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects
Acute toxicity
LD50 Oral - Rat: > 5,500 mg/kg
LC50 - Inhalation - Rat: 4 h - > 12,000 - 20,000 mg/m3
LD50 - Dermal - Rabbit: 12,106 mg/kg
No data available
Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - > 24 h
Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Page 5 of 9
### Respiratory or skin sensitisation
No data available

### Germ cell mutagenicity
- Rat
- DNA damage

### Carcinogenicity
- IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Toluene)
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP
- OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

### Reproductive toxicity
- Damage to fetus possible
- Suspected human reproductive toxicant

### Reproductive toxicity - Rat - Inhalation
- Fetal effects: Spasmotogenic (including genetic material, sperm morphology, motility, and count).
- Experiments have shown reproductive toxicity effects in male and female laboratory animals.

### Developmental Toxicity - Rat - Oral
- Effects on Embryo or Fetus: Teratogenic (except death, e.g., stunted fetus).

### Specific target organ toxicity - single exposure
- No data available

### Specific target organ toxicity - repeated exposure
- No data available

### Aspiration hazard
- No data available

### Additional Information
- RTECS: XG25000000
- Lung irritation, chest pain, pulmonary edema. Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the lungs, trachea, and bronchi in animals. Central nervous system, stomach - irregularities - based on human evidence. Stomach - irregularities - based on human evidence.

### 12. ECOLOGICAL INFORMATION

#### 12.1 Toxicity
- Toxicity to fish: LC50 - Oocythus mykiss (rainbow trout) - 7.8 mg/l - 96 h
- NOEC - Pimephales promelas (fathead minnow) - 5.4 mg/l - 7 d
- Toxicity to daphnia and other aquatic invertebrates: ECO50 - Daphnia magna (Water flea) - 8.0 mg/l - 24 h
- ECO20 - Chironota vulgaris (Freshwater algae) - 245.00 mg/l - 24 h
- ECO20 - Pseudokirchneriella subcapitata (green algae) - 10.00 mg/l - 24 h

#### 12.2 Persistence and degradability
- Biotransformation: Result - Readily biodegradable

#### 12.3 Bioaccumulative potential
- Bioaccumulation: Hexane solution (Golden orla) - 5 d - 0.05 mg/l

### 12.4 Mobility in soil
No data available

### 12.5 Results of PBT and vPvB assessment
- PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects
- An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
- Toxic to aquatic life.

### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods
- Produced
- Burn in a chemical incinerator equipped with an afterburner and scrubber but extra care in igniting as this material is highly flammable. Offer surplus and non-volatile solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of the material.

### 14. TRANSPORT INFORMATION

#### DOT (US)
- UN number: 1294
- Class: 3
- Packing group: II
- Reportable Quantity (RQ): 1000 lbs
- Poison Inhalation Hazard: No

#### IMDG
- UN number: 1294
- Class: 3
- Packing group: II
- EMS-No: F-E, S-0
- Proper shipping name: Toluene

#### IATA
- UN number: 1294
- Class: 3
- Packing group: II
- Proper shipping name: Toluene

### 15. REGULATORY INFORMATION

#### SARA 302 Components
- No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### SARA 313 Components
- The following components are subject to reporting levels established by SARA Title III, Section 313:
  - CAS-No: Revision Date
  - Toluene: 108-86-3 2007-07-01
  - Massachusetts Right To Know Components
    - Toluene: 108-86-3 2007-07-01
  - Pennsylvania Right To Know Components
    - Toluene: 108-86-3 2007-07-01
  - New Jersey Right To Know Components
    - Toluene: 108-86-3 2007-07-01
  - California Prop. 65 Components
    - Toluene: 108-86-3 2007-07-01
16. OTHER INFORMATION

Full text of W-Statements referred to under sections 2 and 3.

Acute Aquatic: Acute aquatic toxicity
Asp. Tox: Aspiration hazard
Flamm: Flammable liquid and vapour.
H225: Highly flammable liquid and vapour.
H304: May be fatal if swallowed and enters airways.
H315: Causes skin irritation.
H335: May cause drowsiness or dizziness.
H361: Suspected of damaging fertility or the unborn child.
H373: May cause damage to organs through prolonged or repeated exposure.
H401: Toxic to aquatic life.
Repr. Toxic: Reproductive toxicity
Skin Irrit.: skin irritation

HMI Rating
Health hazard: 2
Chronic Health Hazard: 2
Flammability: 3
Physical Hazard: 0

NFPA Rating
Health hazard: 2
Fire Hazard: 2
Reactivity hazard: 0

Further Information
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The above information is intended to be correct but does not purport to be all inclusive and shall be used only as a
guide. The information in this document is based on the present state of our knowledge and is applicable to the
product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the
product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling
or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing
slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8650

Version: 5.0 Revision Date: 12/18/2014 Print Date: 02/20/2015
C.10 p-Xylene [40]
4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIGHTING MEASURES
5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self-contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES
6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Wear impermeable protective clothing. Avoid contact with skin and eyes. Keep away from sources of ignition. Use explosion-proof equipment. Keep valve area clear. Keep container closed.

6.2 Environmental precautions
Avoid release to the environment. Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage and then collect with an electrically protected vacuum cleaner or by wet-absorbing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 12.

7. HANDLING AND STORAGE
7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition. No smoking. Take measures to prevent the build up of static electricity. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end uses
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION
8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4-Butanediol</td>
<td>107-53-6</td>
<td>100 ppm</td>
<td>USA, OSHA Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Eye &amp; Upper Respiratory Tract irritation; Central Nervous System impairment; Substances for which there is a Biological Exposure Index or Indices (BEI)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Styrene</td>
<td>(see SEIS section)</td>
<td>Net classifiable as a human carcinogen</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STL</td>
<td>150 ppm</td>
<td>USA, AIHA Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>150 ppm</td>
<td>USA, ACGIH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>150 ppm</td>
<td>USA, OSHA - Table Z-1.1 Limits for All Contaminants</td>
</tr>
</tbody>
</table>

The value in mg/m3 is approximate.

8.2 Exposure controls
Appropriate personal protective equipment.
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment
Eye protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as ANSI Z87.1.
Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove’s outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 400 min
Material tested: V triflare® (KCL 004 / Aidrich 287760, Size M)

Splatter contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 30 min
Material tested: Comfort Fit (KCL 795 / Aidrich 287744, Size M)

Data source: KCL GmbH, D-39124 Eichenzell. Phone +49 (0) 39559 67000, mail sales@kcl.de. Test method: EN574
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the US approved gloves. This recommendation is advisory only and must be evaluated by an

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industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**Body Protection**
Complete suit protecting against chemicals. Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory Protection**
Where risk assessment shows air-purifying respirators are appropriate a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>a) Appearance</th>
<th>Form: liquid, clear</th>
</tr>
</thead>
<tbody>
<tr>
<td>b) Odour</td>
<td>no data available</td>
</tr>
<tr>
<td>c) Odour Threshold</td>
<td>no data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>no data available</td>
</tr>
<tr>
<td>e) Melting point/boiling point</td>
<td>Melting point range: 12 - 13 °C (54 - 55 °F) - lit.</td>
</tr>
<tr>
<td>f) Inst. boiling point and boiling range</td>
<td>128 °C (262 °F) - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>25.0 °C (77.0 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>no data available</td>
</tr>
<tr>
<td>i) Flammability solid, gas</td>
<td>no data available</td>
</tr>
<tr>
<td>j) Flammability or explosive limits</td>
<td>Upper explosion limit: 7 % (v/v)</td>
</tr>
<tr>
<td>k) Vapour pressure</td>
<td>21.3 hPa (100.0 mmHg) at 27.7 °C (81.9 °F)</td>
</tr>
<tr>
<td>l) Vapour density</td>
<td>no data available</td>
</tr>
<tr>
<td>m) Relative density</td>
<td>0.851 gl/cm3 at 20 °C (68.0 °F)</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>0.2 g/l</td>
</tr>
<tr>
<td>o) Partition coefficient n-octanol/water</td>
<td>no data available</td>
</tr>
<tr>
<td>p) Auto-ignition temperature</td>
<td>529.0 °C (984.2 °F)</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>no data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>no data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>no data available</td>
</tr>
<tr>
<td>t) Oxidising properties</td>
<td>no data available</td>
</tr>
</tbody>
</table>

9.2 Other safety information

**Surface tension**
28.3 mN/m at 20.0 °C (68.0 °F)
12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish
LC50 - Oncorhynchus mykiss (rainbow trout) - 2.86 mg/l - 96 h
LC50 - Carassius auratus (goldfish) - 16.00 mg/l - 24 h

Toxicity to daphnia and other aquatic invertebrates
EC50 - Daphnia magna (Water flea) - 35.60 - 63.10 mg/l - 48 h

Toxicity to algae
EC50 - Pseudokirchneriella subcapitata (green algae) - 3.20 - 4.40 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability Result: 87.8 % - Readily biodegradable.

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Toxics to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 1937 Class: 3 Packing group: III
Proper shipping name: Xylene
Repackable Quantity (RU): 100 l/s
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 1937 Class: 3 Packing group: III
EMS-No: F-E, S-D
Proper shipping name: XYLENES
Marine pollutant: No

IATA
Sigma-Aldrich - 29833

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15. REGULATORY INFORMATION

UN number: 1937 Class: 3 Packing group: III

15.1 SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

15.2 SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

p-Xylene
CAS-No. 106-42-3
Revision Date 2007-07-01

15.3 Massachusetts Right To Know Components

p-Xylene
CAS-No. 106-42-3
Revision Date 2007-07-01

15.4 Pennsylvania Right To Know Components

p-Xylene
CAS-No. 106-42-3
Revision Date 2007-07-01

15.5 New Jersey Right To Know Components

p-Xylene
CAS-No. 106-42-3
Revision Date 2007-07-01

15.6 California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Toxicity:
Acute Toxicity
Acute aquatic toxicity
Flammability
Hazardous material
Health hazard
Reactivity hazard
Further information

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C.11 m-Xylene [41]

SIGMA-ALDRICH

SAFETY DATA SHEET

Version 8.0
Revision Date 02/22/2015
Print Date 02/22/2015

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product Identifiers

Product name: m-Xylene

Product Number: 295525
Brand: Sigma-Aldrich
Index-No.: 051-022-00-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich
3650 South Street
SAINT LOUIS MO 63103
USA

Telephone: +1 800-522-8024
Fax: +1 800-522-8023

Emergency telephone number

Emergency Phone #: (314) 776-0550

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS): Flammable liquid (Category 2), H225
Acute toxicity, Dermal (Category 4), H412
Skin irritation (Category 2A), H315
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Aspiration hazard (Category 1), H401
Acute aquatic toxicity (Category 3), H412
Chronic aquatic toxicity (Category 3), H412

For the full list of the H-Statements mentioned in this Section, see Section 18.

2.2 OH&S Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s): Flammable liquid and vapor, Harmful if swallowed and enters always. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. Harmful to aquatic life with long lasting effects.

Precautionary statement(s): Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Keep container tightly closed. Grounding or bonding equipment. DO NOT USE-explosion-proof electrical/ventilating equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Avoid breathing dust/fume/gas/mist/vapors/spray. Wash skin thoroughly after handling. Use only outdoors or in a well-ventilated area. Avoid release to the environment. Wear protective gloves/eye protection/face protection. IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. IF ON SKIN (or hair) Remove/ Take off immediately all contaminated clothing. Rinse skin with water. IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell. IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Do NOT induce vomiting. If skin irritation occurs: Get medical advice/attention. If eye irritation persists: Get medical advice/attention. Take off contaminated clothing and wash before reuse. Do not wash and throw away. Do not store near food - keep cool. Do not use or allow to contact with food - keep cool.

For the full list of the P-Statements mentioned in this Section, see Section 18.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: 1,2-Dimethylnaphtalene

Formula: C10H8
Molecular weight: 138.17 g/mol
CAS-No.: 106-28-3
EC-No.: 203-576-3
Index-No.: 051-022-00-9

Material components

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Xylene</td>
<td>100 %</td>
</tr>
</tbody>
</table>

For the full list of the M-Statements mentioned in this Section, see Section 18.
4. FIRST AID MEASURES

4.1 Description of first aid measures

4.1.1 General advice
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

4.1.2 Inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

4.1.3 In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

4.1.4 In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

4.1.5 If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.

5. FIREFIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon dioxide.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool opened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 12).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition. No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resaled and kept upright to prevent leakage.

7.3 Specific end uses
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Xylene</td>
<td>108-38-3</td>
<td>TWA</td>
<td>100 ppm</td>
<td>USA, NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>150 ppm</td>
<td>USA, NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>100 ppm</td>
<td>USA, Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Remarks</th>
<th>The value in ppm is approximate.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TWA</td>
<td>100 ppm</td>
</tr>
<tr>
<td>STEL</td>
<td>150 ppm</td>
</tr>
</tbody>
</table>

Table 1: Exposure Control Parameters

6.2 Biological exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>m-Xylene</td>
<td>108-38-3</td>
<td>Methlyl IPP</td>
<td>1,500,000</td>
<td>Mouse</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

| Remarks | End of shift (As soon as possible after exposure ceased) |

Table 2: Biological Exposure Limits

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eyes and face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skins protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal techniques without touching glove’s outer surface to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested Mitsuiplast (KCL 880 / Aldrich 2077988, Size M)
Spash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 50 min
Material tested Comatrel® (KCL 710 / Aldrich 2077984, Size M)

Data source: KCL GmbH, D-33124 Bremen, phone +49 (0)521 97730, e-mail sales@kcl.de, test method EN374.

Exposure guidelines
If used in isolation, or mixed with other substances, and under conditions different from EN 374, contact the supplier of the CE-approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use conditions.

Body protection
Complete suit protecting against chemicals. Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the hazardous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose cartridge (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

3. PHYSICAL AND CHEMICAL PROPERTIES

3.1 Information on basic physical and chemical properties
a) Appearance
  - Form: liquid
  - Colour: Colourless
b) Odour
  - No data available
c) Odour threshold
  - No data available
d) pH
  - No data available
e) Melting point/freezing point
  - Melting point/freezing: -48 °C (-64 °F) - lit.
f) Initial boiling point and boiling range
  - 138.0 - 155.9 °C (308.4 - 311.5 °F) - lit.
g) Flash point
  - 25.0 °C (77.2 °F) - closed cup
h) Evaporation rate
  - No data available
i) Flammability (solid, gas)
  - No data available
j) Upper/lower flammability or explosive limits
  - Lower explosion limit: 1.1 % (V)
  - Upper explosion limit: 7.9 % (V)
k) Vapour pressure
  - 8.0 kPa (60 mm Hg) at 20.0 °C (68.0 °F)
  - 21.2 kPa (160 mm Hg) at 37.7 °C (99.9 °F)

l) Vapor density
  - No data available
m) Relative density
  - 0.683 g/ml at 25 °C (77 °F)

n) Water solubility
  - No data available
o) Partition coefficient: n-octanol/water
  - log Pow: 3.2 at 20 °C (58 °F)
p) Auto-ignition temperature
  - 495.0 °C (925.0 °F)
  - 502.0 °C (934.0 °F)
q) Decomposition temperature
  - No data available
r) Viscosity
  - No data available
s) Explosive properties
  - No data available
t) Oxidising properties
  - No data available

3.2 Other safety information
No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Vapours may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
Strong oxidizing agents.

10.6 Hazardous decomposition products
Other decomposition products - No data available

In the event of fire see section 5.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat: male - 9,002 mg/kg (OECD Test Guideline 401)
LC50 Inhalation - Rat - male - 4 h - 6700 ppm
(Directive 97/68/EC, Annex V, B.2.)
LD50 Dermal - Rabbit - male - 12,108 mg/kg
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3,13,2)

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe eye irritation - 24 h

Respiratory or skin sensitisation
- Mouse
12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish: LC50 - Fish - 11.23 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates: Remarks: No data available

Toxicity to algae: Remarks: No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of improper handling or disposal. Harmful to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product: Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in lighting as this material is highly flammable. Other surplus and non-hazardous solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging: Dispose of as unusable product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1907
Class: 3
Packing group: III
Proper shipping name: Xylene
Reported Quantity (RQ): 1000 lbs
Marine pollutant: No
Pnson Inhalation Hazard: No

IMDG

UN number: 1907
Class: 3
Packing group: III
EMS-No: K-E, S-D

IATA

UN number: 1907
Class: 3
Packing group: III
Proper shipping name: Xylene

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

m-Xylene: CAS-No. 108-38-3
Revision Date: 2007-07-01

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

m-Xylene: CAS-No. 108-38-3
Revision Date: 2007-07-01

Pennsylvania Right To Know Components

m-Xylene: CAS-No. 108-38-3
Revision Date: 2007-07-01

New Jersey Right To Know Components

m-Xylene: CAS-No. 108-38-3
Revision Date: 2007-07-01

California Prop. 65 Components
This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.
<table>
<thead>
<tr>
<th>Acute Tox.</th>
<th>Acute toxicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Aquatox.</td>
<td>Acute aquatic toxicity</td>
</tr>
<tr>
<td>Aquatic Chronic</td>
<td>Chronic aquatic toxicity</td>
</tr>
<tr>
<td>Exp. Tox.</td>
<td>Explosion hazard</td>
</tr>
<tr>
<td>Eye Irr.</td>
<td>Eye irritation</td>
</tr>
<tr>
<td>Flam. Liq.</td>
<td>Flammable liquid</td>
</tr>
<tr>
<td>H226</td>
<td>Flammable liquid and vapour</td>
</tr>
<tr>
<td>H304</td>
<td>May be toxic if swallowed and enters airways</td>
</tr>
<tr>
<td>H312</td>
<td>Harmful in contact with skin</td>
</tr>
<tr>
<td>H315</td>
<td>Causes skin irritation</td>
</tr>
<tr>
<td>H310</td>
<td>Causes serious eye irritation</td>
</tr>
<tr>
<td>H335</td>
<td>May cause respiratory irritation</td>
</tr>
</tbody>
</table>

**HMIIS Rating**
- Health hazard: 2
- Chronic Health Hazard: *
- Flammability: 3
- Physical Hazard: 0

**NFPA Rating**
- Health hazard: 2
- Fire hazard: 3
- Reactivity hazard: 0

**Further Information**
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**Preparation Information**
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8906

Version: 5.4
Revision Date: 10/07/2014
Print Date: 02/25/2016
C.12 o-Xylene [42]

SIGMA-ALDRICH
SAFETY DATA SHEET
Revision Date 01/05/2019
Print Date 02/06/2019

1. PRODUCT AND COMPANY IDENTIFICATION
1.1 Product identifiers
Product name: o-Xylene
Product Number: X1040
Brand: Sigma-Aldrich
Index-Nr.: 801-022-00-0
CAS-No.: 108-91-5

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet
Company: Sigma-Aldrich
3060 Grove Street
SAINT LOUIS MO 63102
USA
Telephone: +1 800-325-5632
Fax: +1 800-325-5632

1.4 Emergency telephone number
Emergency Phone #: (314) 770-0555

2. HAZARDS IDENTIFICATION
2.1 Classification of the substance or mixture
GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquid (Category 3), H226
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H314
Skin irritation (Category 2), H315
Reproductive toxicity (Category 2), H361
Acute aquatic toxicity (Category 2), H411
Chronic aquatic toxicity (Category 2), H411

2.2 GHS Label elements, including precautionary statements
Signal word: Warning
Hazard statement(s): Flammable liquid and vapour, Harmful in contact with skin or if inhaled, Causes skin irritation, Suspected of damaging fertility or the unborn child.
Precautionary statement(s): Obtain special instructions before use.

2.3 Hazards not otherwise classified (HINNC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS
3.1 Substances
Chemical characterization: Natural product
Synonyms: 1,2-Dimethylenecyclohexane
Formula: C9H18
Molecular weight: 138.24 g/mol
CAS-No.: 121-77-8
EC-No.: 203-822-2
Index-No.: 801-022-00-9

3.2 Hazardous components
Component: o-Xylene
Classification: Flammable liquid 3, Acute Toxic: 4, Skin Irrit 2, Resp 2
Concentration: >99.0 %

4. FIRST AID MEASURES
4.1 Description of first aid measures
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance.
Inhaled: If breathing is difficult, provide artificial respiration.

Page 1 of 10
In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed
No data available.

5. FIREFIGHTING MEASURES
5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self-contained breathing apparatus for fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES
6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE
7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition. No smoking. Take measures to prevent the build-up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

6. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.915</td>
<td>95-47-5</td>
<td>TWA 100.00000</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td>0.965</td>
<td>95-47-5</td>
<td>STEL 70.00000</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
</tbody>
</table>

Remarks
Eye & Upper Respiratory Tract irritation
Central Nervous System impairment
Substances for which there is a Biological Exposure Index or Indices (see BEI section)
Net classifiable as a human carcinogen

TWA 100.00000 ppm
USA, Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

TWA 100.00000 ppm
USA, NIOSH Recommended Exposure Limits

STEL 70.00000 ppm
USA, NIOSH Recommended Exposure Limits

TWA 100.00000 ppm
USA, Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

The value in mg/m³ is approximate.

TWA 100.00000 ppm
USA, ACGIH Threshold Limit Values (TLV)

Central Nervous System impairment
Upper Respiratory Tract irritation
Eye irritation
Substances for which there is a Biological Exposure Index or Indices (see BEI section)
Net classifiable as a human carcinogen

STEL 70.00000 ppm
USA, ACGIH Threshold Limit Values (TLV)

Central Nervous System impairment
Upper Respiratory Tract irritation
Eye irritation
Substances for which there is a Biological Exposure Index or Indices (see BEI section)
Net classifiable as a human carcinogen
Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological Specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>o-Xylene</td>
<td>78-00-6</td>
<td>Methylnitricetonic acids</td>
<td>1.500 000 0 mg/L</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

Remarks: End of shift (As soon as possible after exposure ceased)

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological Specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methylnitricetonic acids</td>
<td>1.5g/L creatinine</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Remarks: End of shift (As soon as possible after exposure ceased)

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment
Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as ANSI Z87.1 or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove’s outer surface) to avoid skin contact with this product. Disposes of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.2 mm
Breakthrough time: 100 min
Material tested: Vtesse® (KCL 900 / Alene 2977066, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Breakthrough time: 50 min
Material tested: Camflex® (KCL 790 / Alene 2977442, Size M)

Data source: KCL GmbH, D-28124 Emden, phone +49 (0)4858 0760, e-mail sales@kcl.de, test method: EN574

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals. Flame retardant anti-static protective clothing. The type of protective equipment must be selected according to the concentration and amount of the hazardous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or BSI (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. Physical and chemical properties

9.1 Information on basic physical and chemical properties
a) Appearance
   Form: liquid
   Colour: colourless
b) Odour
   No data available
c) Odour threshold
   No data available
d) pH
   No data available
e) Melting point/freezing point
   Melting point: -20 to -23 °C (-15 to -9 °F) - lit
   Freezing point: 143.1 to 145.1 °C (290 to 293 °F) - lit
f) Initial boiling and boiling range
   143.1 to 145.1 °C (290 to 293 °F) - lit
   Flash point: 31.0 °C (87.8 °F) - closed cup
h) Evaporation rate
   No data available
i) Flammability (flash point/pour point)
   No data available
j) Upper/lower flammability or explosive limits
   Upper explosion limit: 6.7 %
   Lower explosion limit: 0.0 %
k) Vapour pressure
   21.3 kPa (150 mmHg) at 37.7 °C (99.9 °F)
   8.8 kPa (66 mmHg) at 25.0 °C (77.0 °F)
l) Vapour density
   No data available
m) Relative density
   0.879 g/cm3 at 20 °C (68 °F)
q) Water solubility
   No data available
r) Partition coefficient: n-octanol/water
   Log Pow: 3.12
p) Auto-ignition temperature
   454.0 °C (857.2 °F)
d) Decomposition temperature
   No data available
f) Viscosity
   No data available
s) Explosive properties
   No data available
t) Oxidizing properties
   No data available

9.2 Other safety information

Surface tension 29.8 mN/m at 25.0 °C (77.0 °F)

10. Stability and Reactivity

10.1 Reactivity
   No data available

10.2 Chemical stability
   Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
   Vapours may form explosive mixture with air.

10.4 Conditions to avoid
   Heat, flames and sparks.

10.5 Incompatible materials
   Oxidizing agents
10.6 Hazardous decomposition products
Other decomposition products - No data available
in the event of fire; see section 6.

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects

Acute toxicity
No data available

Skin corrosion/irritation
No data available

Skin sensitisation
No data available

Reproductive toxicity
No data available

Neural toxicity
No data available

Additional Information
RTECS: ZE2545000

12. ECOLOGICAL INFORMATION
12.1 Toxicity
296
MATERIAL SAFETY DATA SHEET

Product Name: ZSM-5 Zeolite
MSDS No.: Z290604
Effective Date: 01/01/2008
Manufacturer: Qingdao Wish Chemicals Co., Ltd.

SECTION 1. IDENTIFICATION OF PRODUCT

CHINESE NAME: ZSM-5 分子筛
ENGLISH NAME: ZSM-5 Zeolite
CAS No.: 38828-08-5
CHEMICAL: (0.9±0.2) HAlOx·(25-50)SiO₂·2H₂O
FORMULA:

SECTION 2. HAZARD INTRODUCTION

INFECTION PATH: Eyes contact. Skin contact. Inhalation: Ingestion

HEALTH: The material may generate dust in transportation, loading and unloading process. The dust may cause discomfort to eyes, skin, intake and breath. Eyes contact: May cause abrasion or irritation to eyes. Skin contact: Prolonged or repeated contact may dry skin and cause irritation. Inhalation: Dust may irritate respiratory tract and bring temporary or permanent damage (The product contains crystalline silicon that may cause respiratory diseases). Ingestion: May cause damage to digestive system.

SECTION 3. FIRST AID PROCEDURES

SKIN CONTACT: Immediately flush skin with plenty of flowing water while removing contaminated clothing and shoes. Wash clothing before reuse.

EYES CONTACT: Immediately flush eyes with plenty of flowing water or saline for at least 15 minutes, lifting lower and upper lids open.

SECTION 4. FIRE-FIGHTING MEASURES

DANGEROUS: ZSM-5 Zeolite is non-combustible material, no special combustion or explosive property.

EXTINGUISHING Foam, dry chemical or carbon dioxide, sand, water spray.

SECTION 5. ACCIDENTAL RELEASE MEASURES

DISPOSAL: If spills happen, take protective measures to avoid generating dust. Cleaners use appropriate personal protective equipment (SECTION 7). If not polluted, the product can be carefully shoveled or swept up and placed in a suitable container. Keep away from liquid or wet air. If polluted, the product must be cleaned up observing environmental regulations. Avoiding generating dust as possible. Do not allow material to be released to the environment without proper governmental permits, e.g. sewer pipes, public water systems and rivers. A recommendable method is buying the waste in a suitable place ratified by relevant departments. Reuse or combustion of the container is prohibited.

SECTION 6. HANDLING AND STORAGE

HANDLING: Protect the product label. Note cleaning immediately after contact, especially before eating, drinking and smoking.

eyelids occasionally. Get medical attention immediately.

INHALATION: Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention for any breathing difficulty.

INGESTION: If large amounts were swallowed, give large quantities of water to drink, induce vomiting, or use stomach siphon. DON'T GIVE MILK AND FATTY ACID! Call a physician immediately.
SECTION 7. EXPOSURE CONTROLS AND PERSONAL PROTECTION

RESPIRATORY PROTECTION: Use dustproof respirator where dust occurs.

EYE PROTECTION: If necessary, chemical goggles and/or face shield.

BODY PROTECTION: If necessary, protective work clothing.

OTHER PROTECTION: Rubber where contact likely.

OF HANDS: Wash thoroughly after handling. Wash contaminated clothing before reuse.

SECTION 8. PHYSICAL AND CHEMICAL PROPERTIES

Structure sketch of ZSM-5 Zeolite

Figure 1 Framework of ZSM-5 Zeolite (010)

Figure 2 Channels of ZSM-5 Zeolite


PH: Neutral

MELTING POINT: >1600°C

BOILING POINT: Not applicable

HYDROTHERMAL: Structure of zeolite can be kept in a hydrothermal treatment at 700°C in water vapor.

STABILITY: Structure of zeolite can be kept at 1200°C.

PORE SIZE: ~4.8 Å

ODOR: Odorless

CHEMICAL FORMULA: (0.9±0.2)H-Al₂O₃·(25–50)SiO₂·2H₂O

GLUTENOSITY: Non-glutenous

SOLUBILITY: Insoluble in water.

MAIN USES: ZSM-5 Zeolite is mainly used as catalyst for diesel hydrocracking, fixed-bed catalytic cracking. One of the most popular applications of ZSM-5 Zeolite is used as additives of move-bed FCC catalysts and Si/Al ratio is mainly in the range from 40 to 50 (SiO₂/Al₂O₃ molar ratio). In China, ZSM-5 Zeolites with SiO₂/Al₂O₃ molar ratio of 38–42 as additives of FCC catalysts are largely used in reducing alkene content in gasoline. In addition, ZSM-5 Zeolites with a SiO₂/Al₂O₃ molar ratio of 25–30 are used in catalytic cracking of residue in
many countries. Also, ZSM-5 Zeolites are used as
shape-selective catalysts in many reactions, such
as synthesis of diethylbenzene, isomerization of
xylanes, etc.

SECTION 9. STABILITY AND REACTIVITY

STABILITY: Stable under ordinary conditions of use and storage

INCOMPATIBILITIES: Water, Acid and alkaline substance.

CONDITIONS: To air, moisture, light and incompatibilities. AVOID.

SECTION 10. DISPOSAL CONSIDERATIONS

WASTE CHARACTERS: The material can be saved for recovery or recycling.

DISPOSAL: The used material adsorbing organic substance should be stored in a special closed container to avoid spontaneous combustion.

RECOMMENDATION: Don't bury the used material adsorbing organic substance into soil. Don't dump the waste material into public water or river.

SECTION 11. TRANSPORT INFORMATION

RECOMMENDATION: Carefully loading and unloading; Avoid physical damage of package and container; Avoid water (rain and sea water etc.) not to damage the package.