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Direct Route to Phenol from Benzene

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Abstract
Phenol production, expected to exceed 13MM metric tons in 2017, is a significant global industry with many flaws in its current manufacturing method. The Hock process essentially converts high value propylene to low value acetone. The proposed process design, detailed in this report, provides an alternative reaction pathway that utilizes a direct synthesis from benzene, as developed at the Council of Scientific and Industrial Research (CSIR) in New Delhi, India. The endorsed proposal is in accordance with US Patent 8,772,552 B2, that describes the production of phenol via vapor phase oxidation of benzene over a copper chromium oxide catalyst. Environmental protection and worker safety are paramount concerns due to the hazardous nature of phenol and benzene. The inclusion of a ventilation system with flare hoods keeps the concentration of hazardous materials within OSHA guidelines. The design uses air to oxidize benzene within four separate packed-bed reactors with inter-stage coolers. Downstream separation removes non-condensable species, recycles up to 98% of the unreacted benzene, and purifies phenol to design specifications. The plant's capacity is 500MM lb/operating-year of phenol and will be located on the U.S. Gulf Coast as part of an industrial complex. The final product is 99.83% phenol by mass, and contains an aldehyde byproduct as the principal impurity. The design requires an initial investment of $83.6MM, yields a fifteen-year net present value (NPV) of $90M, and has an estimated investor's rate of return (IRR) of 29.2%. The proposed project is forecasted to break-even in Q1 of 2025 immediately following the second year of maximum production capacity. The design is recommended based on project specifications and marketing team projections, though investors should exercise caution with regards to the effect of realistic market data on proposal sensitivities.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

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April 18, 2017

Dear Dr. Sean Holleran and Mr. Bruce Vrana,

Enclosed is a potential design for the industrial production of phenol using the patented process developed at the Council of Scientific and Industrial Research. The proposed plant will be located at an industrial complex on the United States Gulf Coast with benzene available on site and is designed to produce 500MM lb phenol per year at a weight purity of 99.8%.

The CSIR process oxidizes benzene over a copper chromium catalyst to produce phenol in a single step vapor phase reaction without the formation of major byproducts. The proposed design utilizes air as the source of oxygen to reduce cost. The reactions considered in the design release $5.7x10^7$ BTU per hour. The reactor is partitioned into four sections, each separated by a cooler, in an effort to maintain both isothermal and isobaric conditions due to the sensitive nature of the reaction. The considerable heat energy contained in the reactor effluent stream is used for heat integration to pre-heat the reactor feed. The reactor effluent is then further cooled and depressurized using coolers and turbines before being fed to a flash vessel that removes non-condensable species. The liquid exit from the flash is sent to a distillation column to separate benzene and phenol, with the condensed benzene overhead recycled to the beginning of the process. To meet purification specifications, phenol is sent to two additional distillation columns to remove heavy and chemically similar byproducts. Two weeks' supply of phenol is maintained in heated storage tanks.

The plant will operate for 24 hours a day, 330 days a year, with benzene available for $1,100/metric ton and phenol valued at $2,000/metric ton. Our team conducted a thorough analysis of the proposed design to ensure optimal performance and to determine the economic feasibility of the project. Recommendations are included for further enhancement of the process. The proposed design requires an investment of $83.6MM to meet the annual production goal of 500MM lb of phenol, and yields an investor's rate of return (IRR) of 29.2%. We recommend investing in this process while remaining wary of the current phenol market.

Sincerely,

Bryan Daowdat | Gerard David Hoeltzel | Robert Tannenbaum

Direct Route to Phenol from Benzene

Bryan Daowdat | Gerard David Hoeltzel | Robert Tannenbaum

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

Project proposed by Prof. Bruce Vrana.

Department of Chemical and Biomolecular Engineering
School of Engineering and Applied Science
University of Pennsylvania

April 18, 2017

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Section 1

Abstract

Phenol production, expected to exceed 13MM metric tons in 2017, is a significant global industry with many flaws in its current manufacturing method. The Hock process essentially converts high value propylene to low value acetone. The proposed process design, detailed in this report, provides an alternative reaction pathway that utilizes a direct synthesis from benzene, as developed at the Council of Scientific and Industrial Research (CSIR) in New Delhi, India. The endorsed proposal is in accordance with US Patent 8,772,552 B2, that describes the production of phenol via vapor phase oxidation of benzene over a copper chromium oxide catalyst. Environmental protection and worker safety are paramount concerns due to the hazardous nature of phenol and benzene. The inclusion of a ventilation system with flare hoods keeps the concentration of hazardous materials within OSHA guidelines. The design uses air to oxidize benzene within four separate packed-bed reactors with inter-stage coolers. Downstream separation removes non-condensable species, recycles up to 98% of the unreacted benzene, and purifies phenol to design specifications. The plant's capacity is 500MM lb/operating-year of phenol and will be located on the U.S. Gulf Coast as part of an industrial complex. The final product is 99.83% phenol by mass, and contains an aldehyde byproduct as the principal impurity. The design requires an initial investment of $83.6MM, yields a fifteen-year net present value (NPV) of $90M, and has an estimated investor's rate of return (IRR) of 29.2%. The proposed project is forecasted to break-even in Q1 of 2025 immediately following the second year of maximum production capacity. The design is recommended based on project specifications and marketing team projections, though investors should exercise caution with regards to the effect of realistic market data on proposal sensitivities.

Section 2

Introduction & Objective Time Chart

Section 2.1: Introduction

Phenol (C_6H_5OH) is an organic, aromatic compound whose molecular structure is a benzene ring with a single hydroxyl group. The presence of the hydroxyl group results in high polarity which leads to greater affinity for hydrogen bonding with itself and other polar molecules. These chemical properties contribute to phenol's high boiling point of 359 °F. Phenol is a white crystalline solid at room temperature and melts at a relatively high temperature of 105 °F. This physical property is of extreme importance to chemical processes containing this compound since they must maintain high temperatures to avoid solidification.[2.1] The compound is toxic in doses of 1×10^{-6} lb/lb body weight.[2.2]

Phenol is a key chemical intermediate in the commercial production of plastics, nylon, and pharmaceuticals. [2.3,2.4] The Hock, or cumene, process yields phenol and acetone in a mass ratio of 1.5:1. This catalytic alkylation of benzene using propylene currently accounts for 98% of all global production. There are many drawbacks with this method in practice. Propylene production outages in the U.S., due to factory closures by major companies such as ExxonMobil and Dow Chemical, have caused propylene prices to rise more than 100% since Q4 2016.[2.5] Acetone production capacity has also undergone rapid increases and a corresponding decline in demand.[2.6] Under

[2.1] Clark, Jim. "Physical Properties of Phenol." *Chemistry LibreTexts*. N.p., 22 June 2014. Web. 14 Apr. 2017. <https://chem.libretexts.org/Core/Organic_Chemistry/Phenols/Properties_of_Phenols/Physical_Properties_of_Phenol>.
[2.2] "Toxicological Profile for Phenol." *ATSDR's Toxicological Profiles* (2002): Agency for Toxic Substances and Disease Registry, 2015. Web. 2017.
[2.3] U.S. Dept. of Health and Human Services. "Phenol." *Phenol*. N.p., 1989. Web. 14 Apr. 2017. <http://www.eco-usa.net/toxics/phenol.shtml>.
[2.4] Plotkin, Jeffrey S. "What's New in Phenol Production?" *American Chemical Society*. ACS, 21 Mar. 2016. Web. 14 Apr. 2017. <https://www.acs.org/content/acs/en/pressroom/cutting-edge-chemistry/what-s-new-in-phenol-production-.html>.
[2.5] Joarder, Rajiv. "US Propylene Prices Up Over 100%." *Spend Matters*. MINTEC, 13 Feb. 2017. Web. 14 Apr. 2017. <http://spendmatters.com/2017/02/13/us-propylene-prices-100/>.
[2.6] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. 2017.

current market conditions, the conventional reaction converts high value propylene into low value acetone.

The multistep nature of this chemistry results in low selectivity for phenol and is an additional drawback that renders the process reliant on favorable acetone and phenol pricing for profitability. Furthermore, global acetone demand is expected to show decreased growth over the next decade. These complications render the concept of an alternative reaction chemistry to phenol, without the production of low value co-products, extremely intriguing.[2.7,2.8]

There is also a safety concern with this method. The Hock process generates a highly explosive cumene hydroperoxide intermediate with explosion limits between 0.9% and 6.5% volume percent in air and an autoignition temperature of 300 °F.[2.9] The multitude of issues with the Hock process provide the basis for proposal of our team's novel phenol production design. Three years ago in 2014, a research group from the Council of Scientific and Industrial Research (CSIR) in New Delhi, India patented a homogenous, vapor phase, direct reaction pathway for phenol production from benzene using a copper-chromium-oxide catalyst.[2.10] The CSIR's direct route to phenol eliminates the production of acetone while increasing reaction selectivity for phenol. Equation 1 illustrates the irreversible chemical reaction.

<https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.

[2.7] Plotkin, Jeff S. "PERP Program - Phenol, Acetone, Cumene" *Phenol/Acetone/Cumene Production Cost, Process Technology, Supply/Demand*. Nexant, 2013. Web. 14 Apr. 2017. <http://database.thinking.nexant.com/about/cs/news/items/PERP0910_4_Phenol.cfm>.

[2.8] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. 2017. <https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.

[2.9] Cameo Chemicals. "Cumene Hydroperoxide." *CUMENE HYDROPEROXIDE | CAMEO Chemicals | NOAA*. NOAA Office of Response and Restoration, US GOV, 1990. Web. 15 Apr. 2017.

[2.10] US8772552, CSIR, June 2014.

$$C_6H_6 + \frac{1}{2}O_2 \xrightarrow{Cu\text{-}Cr\ Oxide} C_6H_5OH \quad (1)$$

The major competitive advantage of this method over the cumene process is its superior selectivity.[2.11] Our team is considering licensing this technology and will attempt to recreate Rajaram's et. al. findings on a large scale by designing a plant capable of producing 500MM lb phenol/yr with 99% purity by mass. We will attempt to design robust separation techniques capable of handling a wide range of possible byproducts to allow for variations in chemistry. Additionally, our team will analyze the financial viability of such a plant if it were to be operated on the U.S. Gulf Coast with an assumed uptime of 24 hr/day for 330 days/yr. The direct oxidation process presents a tremendous opportunity for economy of operation without an acetone by-product.

[2.11] US8772552, CSIR, June 2014.

Section 2.2: Objective Time Chart

Project Leaders: Robert Tannenbaum, Bryan Daowdat, and Gerard Hoeltzel

Specific Goals:

- Develop a plant with the capacity to generate 500MM lb liquid phenol/yr from benzene via direct oxidation over a Cu-Cr catalyst in accordance with CSIR's patented data
- High product purity and proper disposal of hazardous byproducts should be prioritized

Project Scope:

In Scope:

- Produce 500MM lb liquid phenol per year
- Produce a product with >99% phenol purity by weight
- Determine equipment units needed and corresponding operating conditions
- Determine size and bare module cost of each process unit
- Properly design a reactor capable of carrying out the catalytic reaction
- Determine best methods for disposal of hazardous byproducts
- Analyze the profitability and economics of the process in the context of the assumptions provided in the project prompt along with relevant sensitivities

Out of Scope:

- Further lab work to confirm accuracy of patent data
- Kinetic analysis of patent data
- Manufacture required catalyst
- Test conversion and selectivity assumptions
- Design process control systems

Deliverables:

- Develop complete flowsheet illustrating the designed process with accurate mass and energy balances
- Present a reasonable reactor design for the process
- Provide block results for operating conditions of each unit
- Financial analysis with process and pricing sensitivity analysis

Process Development Timeline:

- Complete mid-semester presentation by Feb. 28th, 2017
- Complete deliverables over the course of the spring semester, with the final polished product complete by Apr. 18th, 2017

Section 3

Innovation Map

N/A

Section 4

Commercial Market & Competitive Analyses

The future market landscape for phenol remains bright despite a drastic increase in global production capacity and decreased demand over the last five years.[4.1] Phenol is most frequently used as a raw material in the production of bisphenol-A (BPA) as a building block for polycarbonate plastic to make DVDs, tablets, flat screen TVs, and mobile phones.[4.2] As the market stands, 46% of phenol sold is used to manufacture BPA. With the expectation that the North American consumer electronics market will grow with a 13.2% compounded annual growth rate and global electronics revenues will more than double from $1.45 trillion in 2015 to $3 trillion in 2020, phenol demand should increase accordingly[4.3]. ICIS agrees, forecasting global demand for phenol to increase at rate of 3% per year for the next decade while claiming decreased growth in the acetone market.[4.4]

Additionally, phenol is required as an ingredient in a range of consumer goods outside of its primary derivative markets. Disinfectants, detergents, and deodorants all require phenol either directly or indirectly. The range of phenolic applications confers a high industrial value on the compound by nature of its versatility.[4.5] Alkylphenols are used to produce surfactants, detergents, and insecticides. Cyclohexanol, a product of phenol hydrogenation, composing 8% of global phenol use, is an intermediate in nylon synthesis.[4.6] Phenol is also used in the pharmaceutical

[4.1] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. <https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.
[4.2] "Versatile Polycarbonate In Different Industries." *Plastics Technology*. Ochre Media Group, 2016. Web. 2017.
[4.3] "Consumer Electronics to Be a US$ 3 Trillion Market by 2020." *Future Market Insights*. N.p., 26 Dec. 2016. Web. 15 Apr. 2017.
[4.4] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. <https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.
[4.5] "Phenol - Uses." *Greener Industry*. EPSRC, The Royal Society of Chemistry, n.d. Web. 15 Apr. 2017.
[4.6] Weber, M., Weber, M. and Kleine-Boymann, M. 2004. Phenol. Ullmann's Encyclopedia of Industrial Chemistry.

industry. Salicylic acid, an intermediate in aspirin production, is produced via the Kolbe-Schmitt process in which liquid phenol and sodium hydroxide are reacted to make sodium phenoxide.[4.7]

In 2010, annual phenol production eclipsed 10 million metric tons, or 20 billion pounds and has increased rapidly over the last five years. The global capacity for phenol in 2017 is estimated to be 13 million metric tons, or 29 billion pounds.[4.8] Analyses of our planned production capacity in the context of these figures predict a total market share of 1.72%.

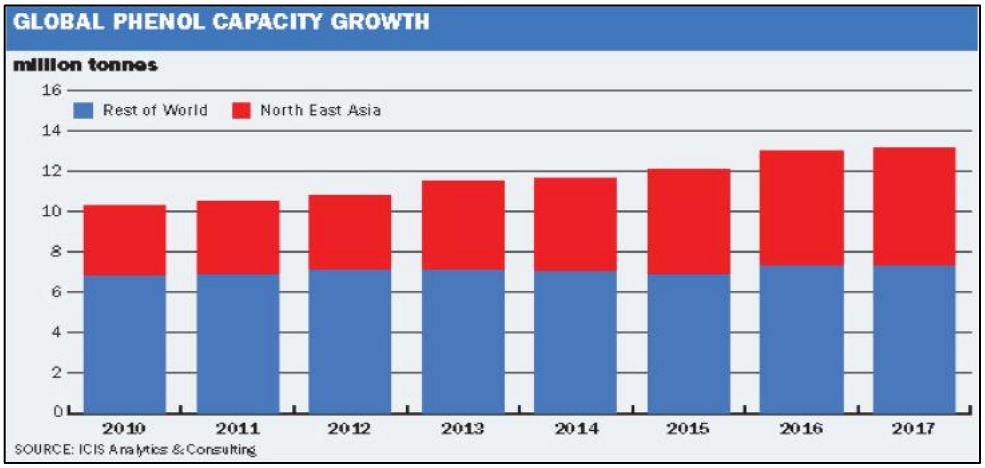


Figure 4.1. Change in global phenol capacity, or total MM tons of phenol produced from 2010 to 2017[4.9].

InspecEthylene OxideSpecialties (INEOS), headquartered in London, stands as the largest incumbent phenol manufacturer, producing more than 4MM metric tons phenol/yr. INEOS has maintained the use of the Hock process for phenol production, taking on the risk of producing an acetone byproduct in stoichiometric proportion to phenol whose value has tended to fluctuate with

[4.7] IHS. "Salicylic Acid 2003 – Chemical Production and Investment Cost." *Information Handling Services*. N.p., Dec. 2003. Web. 15 Apr. 2017.
[4.8] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. <https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.
[4.9] Peacock, Rob. "Market Outlook: Phenol/acetone Markets Are under Pressure: ICIS Consulting." *ICIS.com*. Independent Chemical Information Services, 9 June 2016. Web. 14 Apr. <https://www.icis.com/resources/news/2016/06/09/10006764/market-outlook-phenol-acetone-markets-are-under-ressure-icis-consulting/>.

demand in the petrochemical market.[4.10] The existence of multiple reaction steps in the production of phenol makes it difficult to achieve high phenol yields and correspondingly introduces greater opportunity for undesired products.

Our newly proposed process of producing phenol directly from benzene, using a copper-chromium oxide catalyst with 96.7% selectivity, is a more manageable and economically viable synthetic route for producing phenol. This process poses a serious threat to the incumbent Hock process due to its potential to operate at a much higher margin given the markedly higher selectivity for phenol. Assuming benzene and phenol prices are aligned with those suggested by our marketing team, data from S&P Global Platts estimates a current profit margin of ~10% for the Hock process compared to ~45% for the direct oxidation pathway based on current market prices.[4.11,4.12]

One potential disadvantage in this novel chemistry is the presence of compounds chemically similar to benzaldehyde. Benzaldehyde boils at 353°F and is chemically similar to phenol, which makes for an energetically expensive downstream separation. We chose this compound as a surrogate to model the worst case of potential aldehyde byproducts.

[4.10] "INEOS Phenol." *INEOS Phenol*. INEOS, 2016. Web. 15 Apr. 2017.
[4.11] Staff Reports. "Acetone:US Export Pricing Stable." *S&P Global Platts*. N.p., 2016. Web. 15 Apr. 2017.
[4.12] Joarder, Rajiv. "US Propylene Prices Up Over 100%." *Spend Matters*. MINTEC, 13 Feb. 2017. Web. 14 Apr. 2017. <http://spendmatters.com/2017/02/13/us-propylene-prices-100/>.

Section 5

Customer Requirements

The project objective requires 500MM pounds of phenol to be produced per year. To compete with industry incumbents, high phenol purity is essential. All byproducts produced from the new reactive chemistry are either flushed out or left in trace amounts such that they are unlikely to partake in other phenolic reactions. Industry leaders like INEOS, who utilize the aforementioned Hock process for mass phenol production, sell a range of technical phenol grades varying from 85-99.9 wt % phenol with water composing the remaining mass.[5.1] As the largest producer of technical grade phenol, INEOS's product purity represents the industry standard.

Sigma-Aldrich, a subsidiary of Merck, produces a reagent grade phenol product with weight specifications ranging from 89% phenol with 10% water and 1% unspecified impurities to personalized phenol orders consisting of 99% phenol with 1% unspecified impurities.[5.2]

The proposed process generates a final product with 99.83% purity by mass. Benzaldehyde is the main impurity and composes 0.168% of the final product by mass. A key consideration for our final product, compared to those sold by other producers, is the novel reactive chemistry, which is responsible for producing an aldehyde byproduct. Because 98% of production plants use the same process, purity levels between technical grade phenol have little variation.

The direct route to phenol via benzene oxidation over a copper chromium catalyst produces a new phenol product given the assumed impurities. It should therefore be treated as such, with acknowledgment that reaching the same product specifications as a process with distinctly different chemistry is physically impossible. The chemistry of this reactive pathway assumes the production of small amounts of aldehydes as well as organic acids. A final liquid product purity

[5.1] "INEOS Phenol." *INEOS Phenol*. INEOS, 2016. Web. 15 Apr. 2017.
[5.2] "Reagent Grade Phenol." *Phenol*. Sigma-Aldrich, 2017. Web. 15 Apr. 2017.

of 99.83% by weight positions our product well towards the forefront of the phenol production industry.

The developed process design marginally surpasses the project goal and is capable of generating 505MM lb of liquid phenol per year. Slight overproduction was accounted for in case a small amount of phenol is lost elsewhere in the process; this loss was not accounted for in the ASPEN process simulation.

The proposed design specifically produces liquid phenol to meet the most common phenol customer requirements: industrial manufacturers seeking to use phenol in the production of bisphenol-A, alkylphenols, salicylic acid, phenol formaldehyde resin, and a wide range of additional phenolic resins. Phenol alkylations are carried out predominantly in the liquid phase as are condensation reactions involving phenol such as the production of Bisphenol-A.[5.3]

[5.3] Fiege, H., Voges, H.-W., Hamamoto, T., Umemura, S., Iwata, T., Miki, H., Fujita, Y., Buysch, H.-J., Garbe, D. and Paulus, W. 2000. Phenol Derivatives. Ullmann's Encyclopedia of Industrial Chemistry.

Section 6

Critical-to-Quality (CTQ) Variables

Section 6.1: Reactor Temperature, Pressure, and Pressure Drop

The optimal reactor conditions were determined from patented data to be 662 °F and 580 psig[6.1]. Deviations from these conditions prove to significantly decrease selectivity for phenol while increasing benzene conversion. The combination of these two phenomena drastically decrease phenol yield, increase the presence of unwanted byproducts, and waste valuable benzene feedstock. Concern over maintaining optimal reactor conditions emerged from our desired product purity goal of greater than 99% phenol by mass. Additionally, an increase in conversion and decrease in reaction selectivity would increase the energy requirements on downstream separation processes. Specific reaction data can be found in Tables 1 and 3 in Appendix 2, pgs. 154 and 155.

Patented data indicates that reaction conversion is greatly affected by extreme changes in pressure. However, under the current design, the pressure drop through each reactor vessel is 2.14 psi. This value is low enough to assert that pressure drop through each reactor bed is insignificant to process quality.

Section 6.2: Unreacted Benzene Recovery

Given the low benzene conversion for the reaction, the percent of unreacted benzene recovered in the recycle stream was a crucial variable for project value. A detailed sensitivity analysis of the impact of this variable on project net present value (NPV) can be found in Section 20, pg. 130. Downstream separation vessels were optimized to recover as much benzene as possible because profitability is dependent on a greater than 78.4% unreacted benzene recovered.

[6.1] US8772552, CSIR, June 2014.

Section 6.3: Phenol Product Purity and Production Capacity

To generate a competitive phenol product, final purity must be at least 99% phenol by mass. This desired mass composition along with our production goal of 500MM lb phenol/yr were requirements for the final process and necessitated the development of more rigorous downstream separation techniques. The operating conditions for each process unit were determined using these goals as guidelines.

Section 6.4: Phenol Storage Temperature

It is also of critical importance that our final product be stored at a temperature above its high melting point of 105 °F to avoid phenol solidification. Our team designed a heated storage tank complete with a pump-around heat exchanger to maintain the necessary temperature requirements for liquid phenol. This pump-around should be designed with a process control unit to ensure liquid phenol stability regardless of seasonal temperature variations.

Section 7

Product Concepts

N/A

Section 8

Superior Product Concepts

N/A

Section 9

Competitive Patent Analyses

As previously mentioned, the Hock process is the most widely used method to produce phenol. The synthesis is reliant on the oxidation of cumene to cumene hydroperoxide. The synthesis of benzene through this method requires the alkylation of benzene by isopropanol or propylene, which yields cumene that is oxidized to cumene hydroperoxide and undergoes acid cleavage to produce major products phenol and acetone.[9.1] The principal issues with the conventional phenol production pathway are the presence of acetone as the major byproduct and the low yield of phenol. The annual growth rates for acetone and phenol are estimated to be 2% and 3%, respectively, through the next decade.[9.2]

The Hock process also presents chemical and safety concerns as both the oxidation of cumene and the acid cleavage of its hydroperoxide derivative are highly exothermic reactions. While the proposed process is also exothermic, the reactivity of benzene is less than that of cumene, as seen by their lower and upper explosion limits (LEL, UEL). For benzene, the LEL and UEL are 1.3 and 7.9 % by weight respectively. For cumene, the LEL and UEL are 0.9 and 6.5 % by weight. To handle the formation of cumene and cumene hydroperoxide, reaction and design equipment would need to be more expensive to guarantee worker safety.

Forecasted growth in the phenol market is a result of of rising demand for the main phenol derivative BPA. This surge in demand is attributable to the versatility of BPA as it is used to produce polycarbonate plastics and epoxy resins. Polycarbonate is valuable due to its lightness and its high thermal, impact, and electrical resistance. Polycarbonate plastics are used across a plethora of industries. Eyeglass lenses, police visors, sports helmets, vehicles, medical devices, food

[9.1] PERP Program, Nextant, 2013, http://database.thinking.nexant.com/about/cs/news/items/PERP0910_4_Phenol.cfm.
[9.2] American Chemical Council, Henteges Steve, February 2014 http://factsaboutbpa.org/benefits-applications/why-bpa.

containers, electronic casings, and media discs can all be made with polycarbonate plastic.[9.3] Epoxy resins are a type of thermoset plastic known to exhibit high impact and chemical resistance along with strong adhesion. Epoxy resins are used to create wind turbine blades, electrical equipment, vehicle and metal coatings, aerospace equipment, and marine equipment. More uses for BPA are still being discovered, indicating that its global demand will continue to increase. Because the production of BPA requires phenol and acetone in a 2:1 molar ratio, growth in the phenol market has tended to outpace that of acetone[9.4]. The difference in stoichiometric quantities limits the market value of acetone, as phenol producers will have a surplus of low-value acetone. Despite being introduced in 1944, the main reason that the Hock process remains the principal process is the lack of a viable alternative reaction pathway.

Since the mid-20th century, patents pertaining to phenol production have primarily focused on improvements to the current process rather than an alternative. One example is a European patent filed by Mitsui Petrochemical LTD in 1989. The patent application proposed a method to reduce the acetone byproduct through the integration of a recycle loop.[9.5] The recycle stream, containing acetone separated from phenol, is hydrogenated to isopropanol, then returned to the reactor for benzene alkylation. This patent would reduce the operating cost, as less isopropanol would be needed to achieve similar yields.

Another example is a patent filed in 2003 to increase the efficiency of phenol separation from a cumene mixture. The patent was intended to improve upon the downstream separation of a

[9.3] American Chemical Council, Henteges Steve, February 2014 http://factsaboutbpa.org/benefits-applications/why-bpa.
[9.4] Plotkin, Jeff S. "PERP Program - Phenol, Acetone, Cumene" *Phenol/Acetone/Cumene Production Cost, Process Technology, Supply/Demand*. Nexant, 2013. Web. 14 Apr. 2017.
[9.5] EP0371738A2, Mitsui Petrochemical Industries, November 1989.

variation of the Hock process that increases phenol yield while decreasing operational and utility costs.[9.6]

To avoid potential cumene-related issues, research sought to oxidize something other than cumene. Shell Corp. filed and published a patent in 2005 to produce phenol through the oxidation of s-butylbenzene. The principal advantage of Shell's process is that the acid cleavage of s-butylbenzene hydroperoxide produces methyl ethyl ketone (MEK).[9.7] The patent also contains data to produce phenol by oxidizing a mixture of s-butylbenzene and cumene. MEK can be used as a lacquer or resin solvent, and has a higher commercial value than acetone despite lower demand. Chemically, both MEK and acetone have similar properties, but MEK is considered a specialty chemical. Shell acknowledges this constraint by outlining a proprietary process that oxidizes a mixture of certain alkylbenzenes which can be adjusted to meet demand requirements of MEK.[9.8]

No true alternative route for producing phenol was found until ExxonMobil patented a process in 2010 that produced phenol and cyclohexanone from benzene without the use of isopropanol or propylene. ExxonMobil's patented process claimed to increase phenol yield, produce a co-product that is in high demand in cyclohexanone, and improve the overall safety of phenol production. Principal advantages of this process include the absence of propylene, which is growing more expensive, and the production of cyclohexanone. Cyclohexanone has high industrial demand for its uses as a solvent, lacquer, additive to lubricating oil, and as an intermediate for nylon production.[9.9] Due to ExxonMobil's presence in industry, cyclohexanone is especially valuable as it can be used within the company and the surplus can be sold for a profit.

[9.6] US6583326B2, June 2003.
[9.7] WO200407423OA1, Shell Corporation, November 2005.
[9.8] WO2010098916A2, ExxonMobil, September 2010.
[9.9] National Center for Biotechnology Information. PubChem Compoud Database; CID=7697, https://pubchem.nchi.nih.gov/compound/7967.

The development of such a process presents a considerable market advantage, but the issue of a co-product and costly separation persists.

In 2012, a group of researchers from CSIR filed to patent a process that produces phenol from benzene in a direct route without any major co-products. The patent was published in June of 2014, and presents a number of advantages from a chemical standpoint. The process is composed of a single step, utilizes one catalyst, results in desirable yield, and produces no significant or dangerous byproduct.[9.10] The CSIR team's process uses air to oxidize benzene over a Cu-Cr oxide catalyst. The use of a single catalyst with significant longevity presents an opportunity to reduce the cost of phenol production. This report's goal is to determine the economic viability of this process under conditions derived from the patent.

[9.10] US8772552, CSIR, June 2014.

Section 10

Preliminary Process Synthesis

Section 10.1: Initial Considerations

Benzene is a major chemical product derived from petroleum that is typically used to produce phenol. The conventional process used to produce phenol first requires the production of cumene through the alkylation of benzene with propene or isopropanol over a zeolite acid catalyst:

$$C_6H_6 + C_3H_6 \rightarrow C_9H_{12} \quad (2)$$

Cumene is then oxidized to produce cumene hydroperoxide:

$$C_9H_{12} + O_2 \rightarrow C_9H_{12}O_6 \quad (3)$$

Cumene hydroperoxide undergoes acidic cleavage to produce phenol and acetone:

$$C_9H_{12}O_2 \rightarrow C_6H_5OH + C_3H_6O \quad (4)$$

Figure 10.1 shows the current cumene-based phenol synthesis.

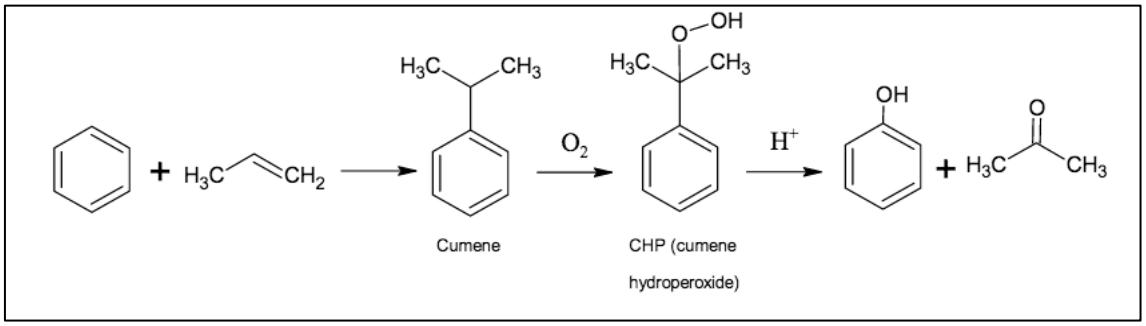


Figure 10.1: Equations (2) through (4) are depicted. The current indirect route is flawed, as the profitability of the process is dependent on the cost of propene and the value of acetone. The demand for propene is rising faster than supply, which will increase the price of propene for the near future. The markets for both phenol and acetone are growing, but due to the large supply of acetone it is not a valuable co-product.

The CSIR research group proposes a single-step vapor oxidation of benzene with air over a Cu-Cr catalyst to produce phenol with no major byproducts. The project goal is to optimize the CSIR process to produce 500MM lb/year of phenol and determine economic feasibility. The project statement provided multiple assumptions. The process will be run at a plant complex on the United States Gulf Coast, the Cu-Cr oxide catalyst is purchased from a vendor, liquid benzene

is available on site for $1,100/metric ton, and phenol is valued at $2000/metric ton.[10.1] Industrial consultants recommended a plant uptime of 330 days/yr, 24 hr/day. The minimum phenol production rate needed to meet the yearly goal is 63,100 lb/hr. Project profitability requires a fresh benzene feed flowrate less than 115,000 lb/hr, based on pricing assumptions from our marketing team.

To realistically model the process, byproducts of catechol, benzoic acid, and benzaldehyde are assumed. Benzoic acid and benzaldehyde model potential categories of byproducts from the under-oxidation of benzene. The formation of cyclohexadiene-aldehyde and hexadiene-acid is more likely; however, benzoic acid and benzaldehyde have boiling points similar to these compounds and have thermodynamic data present in the ASPEN Database. The close boiling points of these assumed byproducts require a more robust downstream separation. The development of rigorous separation units allows the proposed process to remove byproducts with greater relative volatilities than those assumed to allow for slight variation in process chemistry. Benzene polymerization is also a possibility, leading to the formation of relatively dense hydrocarbons. If complete combustion were to result in the formation of carbon dioxide, downstream removal of non-condensables is rigorous enough to handle it. Due to the high reaction temperature and pressure, we ensured that the mass concentration of oxygen in the reactor was less than 5% to avoid explosion limits. Catechol served as a model for the product of benzene over-oxidation, as previous research reported its presence in benzene oxidation. Table 10.1 shows all the reactions modeled in the design.

[10.1] Direct Route to Phenol from Benzene, Suggested Design Projects, Bruce M. Vrana.

Table 10.1: The reactions modeled, their fractional conversion in percent, and product(s) produced are shown. Values for conversion are taken from the patent and estimated using an RGIBBS reactor in ASPENPlus9 at reaction conditions. Combustion produces water and carbon dioxide, if not modeled in table, production is trace. The heats of reactions included are calculated using ASPEN data and fractional conversion.

Reaction	**Product(s)**	**Fraction Conversion [%]**	$\Delta H_{reaction}$ **(BTU/hr)**
$C_6H_6 + \frac{1}{2}O_2 \rightarrow C_6H_5OH$ (1)	Phenol	12.100	-5.4x10^7
$7C_6H_6 + \frac{15}{2}O_2 \rightarrow 6C_7H_6O_2 + 3H_2O$ (5)	a. Benzoic Acid b. Water	0.025	-3.9x10^4
$7C_6H_6 + \frac{9}{2}O_2 \rightarrow 6C_7H_6O + 3H_2O$ (6)	a. Benzaldehyde b. Water	0.025	-1.9x10^4
$C_6H_6 + O_2 \rightarrow C_6H_6O_2$ (7)	Catechol	0.350	-3.1x10^6

The contents of Table 10.1 reflect assumptions and information from the CSIR patent. Reaction conditions were determined to be 662 °F and 580 psig. At these conditions, the patent provides data for benzene conversion, phenol yield and selectivity at various liquid hourly space velocities (LHSV). The LHSV of benzene is given in units of $[\frac{mL\ benzene}{hr*g_{catalyst}}]$, where mL benzene is assumed to correspond to total volumetric flow through our reactor. An LHSV of 100 $\frac{mL\ benzene}{hr*g_{catalyst}}$= 1.60 $\frac{ft^3\ benzene}{hr*lb_{catalyst}}$ matches with a 12.5% conversion of benzene, 12.1% yield of phenol, and selectivity of 96.7%. The LHSV chosen gives low conversion but high selectivity. High selectivity is preferable as it reduces the amount of impurities in the process while low conversion requires high benzene recovery for an optimal process design. A higher value for LHSV could have been chosen to improve selectivity, but would result in significantly lower conversion of benzene. High conversion occurs at low LHSV but is unrealistic to meet the design goal of 500MM pounds. The low conversion at reaction conditions indicates that a sizable recycle stream of unreacted benzene

is necessary and will be an important design consideration. The viability of the CSIR process depends on the amount of unreacted benzene recovered. The heat of reaction data in Table 10.1 is calculated using information from ASPEN. The block report for the reactor calculated the heats of reactions per lbmol and the extents of reaction from the fractional conversion. All reactions included are exothermic and the high amount of heat released is an important design consideration. Due to the elevated levels of temperature and pressure in the reactor, certain heat exchangers will require heating oil as a heat transfer media, as later discussed in Section 14, pg. 65. Heating oil is able to withstand elevated temperatures without undergoing any phase change, unlike cooling water which would likely form a steam envelope and inhibit the transfer of heat.

The difference between conversion and yield indicates the presence of multiple reactions. The possible concentrations of significant products in the side reactions were determined using an RGIBBS reactor in ASPEN. This analysis led to the assumption that carbon dioxide would not be a major byproduct of this process. As previously mentioned, in the event that this assumption is proven wrong in practice, the downstream separation is robust enough to handle the presence of an additional non-condensable chemical. Exact mass flow rates were determined with information from the project statement and the patent. The presence of NO_2 was initially assumed, but after an RGIBBS analysis, it was excluded due to a reaction temperature below 1000 °F.

The size of all equipment included in the process needs to account for transportation, meaning that no piece should be wider than 18 ft, the average roadway width in the United States. Both phenol and benzene are highly toxic, even at low concentrations. The design of the process must employ proper safety considerations, such as a flare system, to meet or exceed all environmental standards.

Section 10.2: Separation

To ensure effective separation, all components of the process were investigated for the presence of azeotropes. Due to the low conversion of benzene in the process, benzene-phenol interactions were also considered. The Journal of Chemical and Engineering Data provides evidence that phenol and benzene do not form an azeotrope.[10.2] Interactions with water were also considered due to its presence as a byproduct. Water exhibits an azeotrope with both benzene and phenol, but the mole fraction of water in the process is well below the azeotropic value.[10.3] The assumed production of benzaldehyde in the process presents a potential problem, as an azeotrope with phenol forms at 366 °F.[10.4] The concentration of the aldehyde product in the process is not high enough to form an azeotropic interaction but presents a separation issue due to its comparable boiling point. Phenol boils at 359 °F while benzaldehyde boils at 353 °F under ambient pressure. The benzaldehyde is a detriment to the purity of phenol produced.

In the single-step synthesis of phenol from benzene, air is the oxidizing agent, resulting in the presence of unreacted oxygen and nitrogen along with the byproducts of benzoic acid, benzaldehyde, catechol, and water in the reactor effluent. Full conversion of oxygen is improbable. Industrial consultants recommended using a conversion around 90% for a more realistic design.

In preliminary design, the reactor effluent was fed directly into an absorption column to separate non-condensables and organics. The organic stream entered a distillation column with two liquid outlets and one vapor outlet. The vapor stream contained a significant amount of benzene and was recycled to the reactor. The liquid stream taken off the condenser contained the

[10.2] Journal of Chemical & Engineering Data, Vol. 43, No. 6, Neinhaus et.al, 1998.
[10.3] Azeotropic Data for Binary Mixtures, University of Oregon, 2014.
[10.4] ChemIndustry, 2010, http://chemindustry.ru/Benzaldehyde.php.

non-condensables with small amounts of benzene and phenol. The bottoms liquid product stream was split, with one partition cooled and returned to the absorption column, and the other to be further processed. The cooled liquid stream returned to the absorption column to function as both a solvent that strips vapor phenol from the reactor effluent, and a coolant that reduces outlet temperature. The preliminary process can be seen in Figure 10.2.

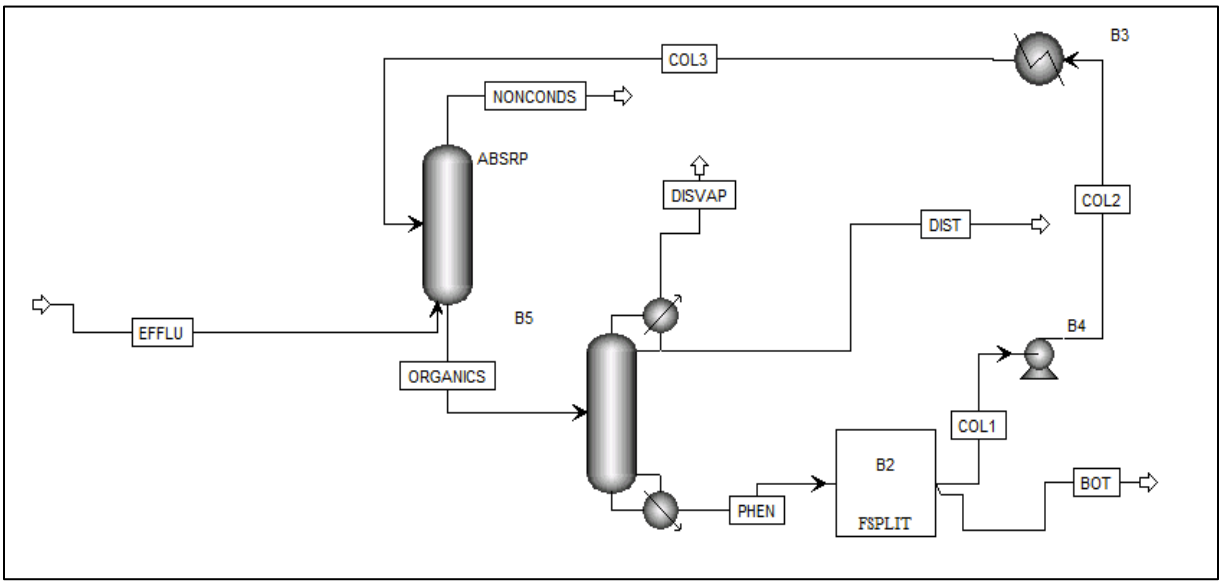


Figure 10.2: Preliminary Process Flow Diagram. Shown is a preliminary design consideration consisting of an absorption column and a distillation column as the main separation vessels.

The absorption column was effective in removing the non-condensable species and the distillation column in separating benzene and phenol, but there were several drawbacks to this design. The need to feed cooled phenol to the absorption column created an additional recycle loop and a more complex design problem. The separations occurred at high temperature and pressure, resulting in extreme downstream operating conditions and large energy requirements. We realized that the inclusion of valves and heat exchangers prior to the downstream processes could allow for more moderate separation conditions. The preliminary design shown needed an additional distillation column to further purify phenol to meet customer requirements. The use of an

absorption tower was expensive and ultimately deemed unnecessary. The purpose of the absorption column was to remove volatile impurities, and can be accomplished by alternatively using a flash drum. The use of a flash drum removes the need for a recycle loop and significantly reduces cost.

The first separation event in the final design uses a flash drum to exploit volatility differences between non-condensables and heavier reaction products to remove gaseous species. Similar to the absorption column, the flash drum removes most of the nitrogen and unreacted oxygen, but some of the benzene is present. Current design conditions remove 90.6% nitrogen by weight with the flash drum. The removal of nitrogen is necessary to ensure that further downstream separation vessels are of reasonable size, as the nitrogen has the highest volumetric flow. Three distillation columns are used, the first to achieve separation between benzene and phenol. The second column separates phenol and catechol. The benzene stream from the first column is recycled to the beginning of the process. The amount of unreacted benzene recycled was determined using the prices of benzene and phenol given. For a profitable process, 85% of unreacted benzene needs to be recycled. This value does not include any process or equipment cost, meaning that the percent recycled will only increase. The third column purifies phenol from benzaldehyde to meet customer purity specifications of 99.8% by mass. Catechol is repurposed within the process as fuel to the furnace. Downstream columns are operated at close to ambient pressure to ensure reasonable equipment costs. The similar boiling points of phenol and benzaldehyde result in an undesirable amount of benzaldehyde in the purified phenol. The choice of benzaldehyde as a byproduct may not be realistic, but its similarity to phenol requires a more rigorous separation than may be needed. The performance of the distillation columns are meant to account for various non-condensable species not explicitly mentioned in the proposed design.

Section 10.3: Reactor Considerations

Liquid benzene is available on site and will require a significant amount of energy to reach reactor conditions. Similarly, the air fed to the process needs to be compressed to reach reactor conditions. The reactions included in the direct synthesis release over 5.7×10^7 BTU/hr, which was used to develop a heat exchanger network in which the reactor effluent pre-heats the reactor feed. The thermal energy capable of being transferred from the reactor effluent is not sufficient to fully heat the reactor feed but decreases utility costs.

The size of the reactor depends on the stoichiometry of the reactions, shown in equations (1), (5) to (7), and the mass of the catalyst. The LHSV of 100 $\frac{mL\ benzene}{hr*g_{catalyst}}$ =1.60 $\frac{ft^3\ benzene}{hr*lb_{catalyst}}$ is used to determine the mass of catalyst required, along with the pressure drop in the reactor and its diameter, as detailed in Section 15.1.3, pg. 76.

Based on the information in the patent, the process is sensitive to temperature, as selectivity declines sharply above 662 °F (Appendix 2, pg. 154). To account for the change in separation due to the products of common side reactions not included, the columns are designed to remove all potential impurities dissimilar to phenol, as modeled with the inclusion of benzaldehyde. Separate reactor vessels with intercoolers were designed in an effort to keep the reactor vessels reasonably isothermal. The temperature rise in the vessel was determined by setting the heat duty of the reactor to 0 BTU/hr and recording the corresponding adiabatic temperature rise. The number of reactor vessels was determined from this overall temperature increase and by assuming a permissible temperature fluctuation of 54 °F per reactor unit.

Section 11

Assembly of Database

Section 11.1: Input Costs

To produce phenol with the CSIR process, benzene and oxygen are required as feedstocks. The project statement provides a benzene purchasing cost of $1,100/metric ton and a selling price of phenol to be $2,000/metric ton. To reduce variable costs, ambient air was used as the source of oxygen. Water and steam prices were taken from Chapter 17 of *Seider et. al, 2017*. To meet safety standards and improve heat integration strategy, we employed the use of a flare system and hot oil furnace. The flare and furnace use natural gas for fuel. Its market price was taken from Bloomberg Energy.

Section 11.2: ASPEN Simulation

Our team used ASPEN Plus v9 to simulate the entire design process. Initially, the non-random two-liquid model (NRTL) was chosen to account for potential azeotropes. Early simulations confirmed that the low amount of water would not cause great separation difficulty. To improve the thermodynamic data for chemically similar hydrocarbons, the Peng-Robinson model was used. Gaseous interactions were considerable because the CSIR process is a vapor-phase oxidation. The Peng-Robinson equations of state, compared to other models, more accurately predict the behavior of chemical species near their critical points.

The design process used a single RSTOIC block to model the total reactor scheme. Heaters, turbines, and compressors were used to account for temperature and pressure changes. A HEATX block was used to model the main exchanger for heat integration. The distillation columns were modeled with RADFRAC blocks. The initial inputs for the RADFRAC blocks were estimated using DSTWU blocks. RADFRAC blocks were necessary to more accurately model separation

events because they perform more rigorous calculations than DSTWU to account for components in small concentrations.

Operating conditions for the distillation columns were determined through the use of design specifications to ensure phenol purity while also optimizing reflux ratio. To improve efficiency and reduce utility costs, all separations were conducted close to ambient pressure.

Benzene is a highly toxic substance and known carcinogen. OSHA regulations state that a concentration greater than 500 ppm poses immediate danger to life and recommends a peak concentration of no more than 50 ppm.[11.1] Phenol is also toxic, with OSHA regulating exposure to 5 ppm.[11.2] Environmental discharge is highly discouraged for both benzene and phenol. The hazardous nature of these chemicals inspired the inclusion of a flare system to combust benzene and a storage tank for phenol.

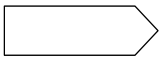
[11.1] Benzene SDS, Chevron Phillips, 2016.
[11.2] Phenol SDS, Sigma Aldrich, 2016.

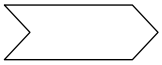
Section 12

Process Flow Diagrams & Material Balances

Section 12.1: General Process Definitions

Ambient Conditions: 86 °F and 0.0 psig
Reaction Conditions: 662 °F and 580.1 psig
High Pressure Steam (hps): 500 psig
Low Pressure Steam (lps): 15 psig
Heat Transfer Media (htm): Heat transfer oil[12.1] with cp= 0.645 BTU/(lb-°F)
Cooling Water (cw): available at ambient conditions
Boiler Feed Water (bfw): available at the saturation point of 15 psig steam

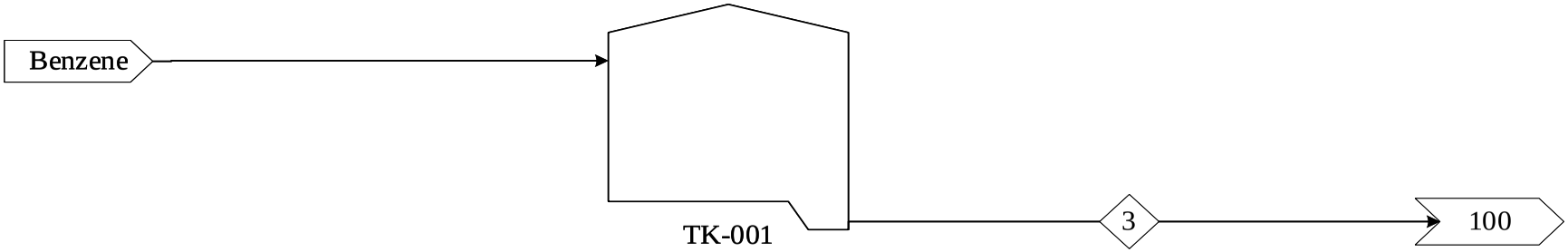
 refers to a stream entering or leaving the entire process

 refers to a stream moving between different process sections

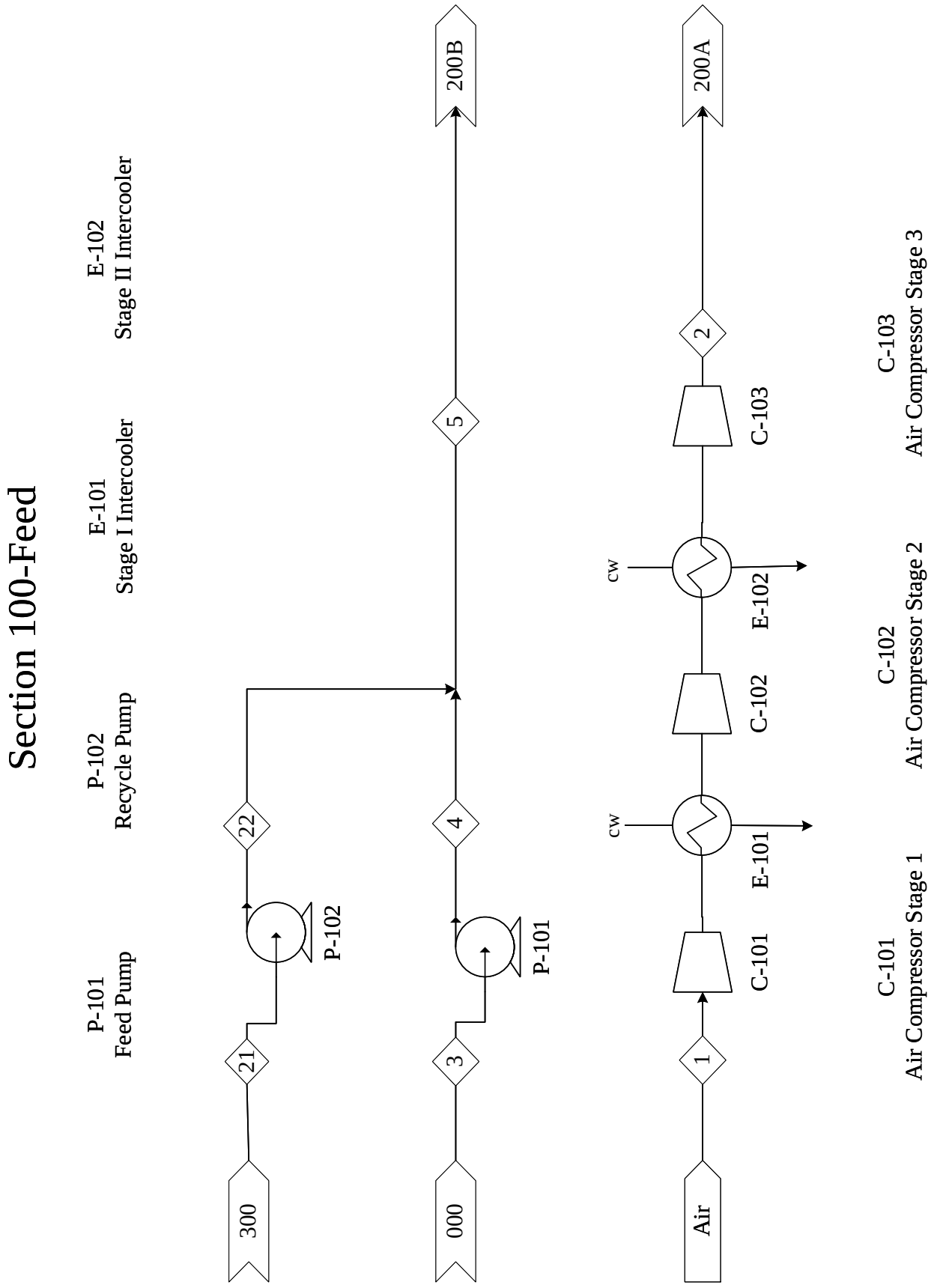
[12.1] Shell Heat Transfer Oil S2 TDS, Shell Corp, August 2010.

Section 000-Feed Storage

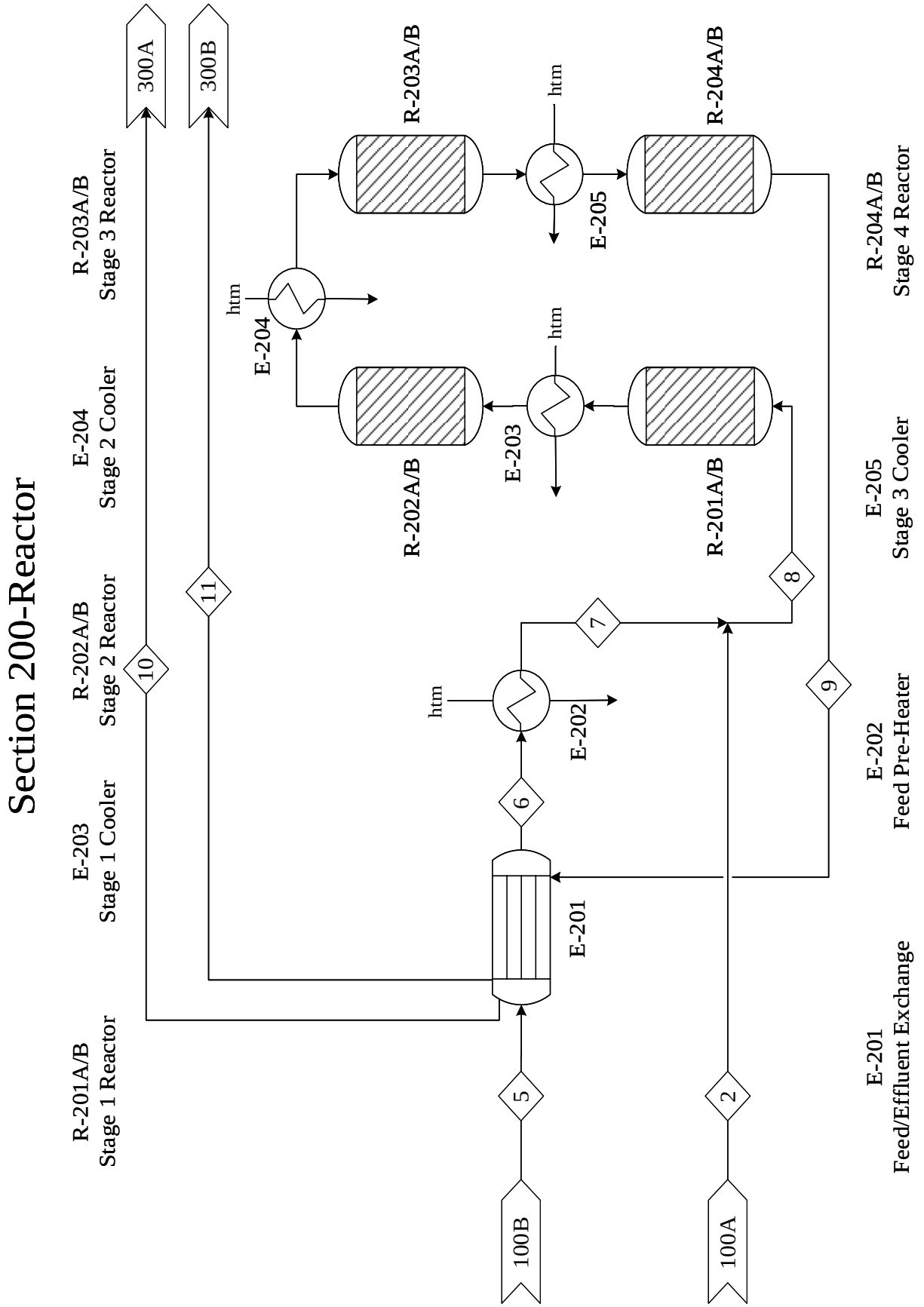
TK-001
Benzene
Storage Tank



Stream Number	3
Temperature (°F)	86
Pressure (psig)	0.0
Vapor Fraction	0.0
Mass Flow (lb/hr)	65616
Component Mass Flow (lb/hr)	
Benzene	65616
Phenol	-
Catechol	-
Benzoic Acid	-
Benzaldehyde	-
Water	-
Oxygen	-
Nitrogen	-
Molar Flow (lbmol/hr)	840
Operating Volume Flow (cuft/hr)	1212

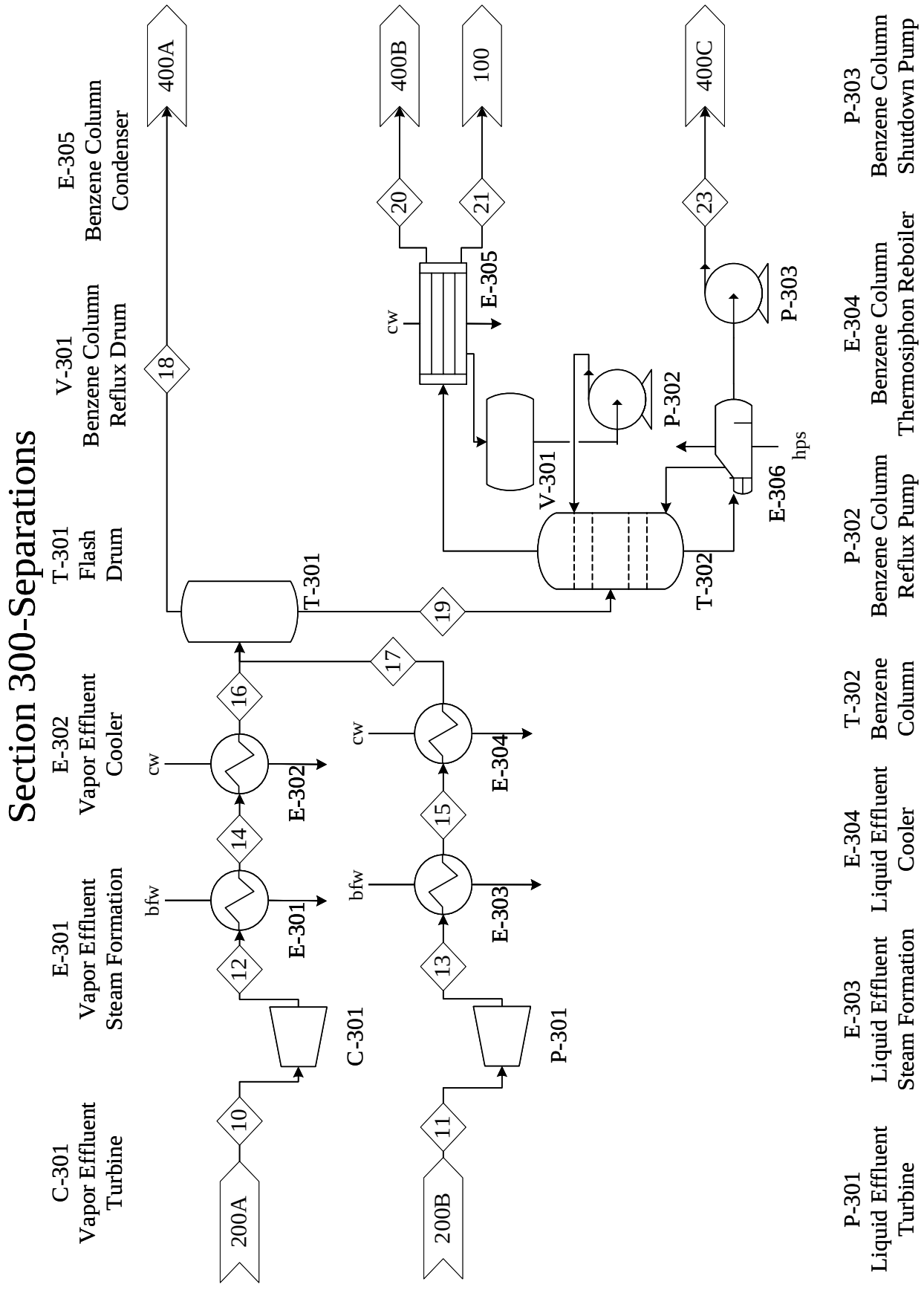

Section 100-Feed
P-101
Feed Pump
P-102
Recycle Pump
E-101
Stage I Intercooler
E-102
Stage II Intercooler
C-101
Air Compressor Stage 1
C-102
Air Compressor Stage 2
C-103
Air Compressor Stage 3
300
000
Air
200B
200A
21
22
3
4
1
2
5
P-101
P-102
C-101
C-102
C-103
E-101
E-102
CW
CW

Stream Number	1	2	3	4	5	21	22
Temperature (°F)	86	384.1	86	92.1	165	172.4	176.6
Pressure (psig)	0.0	580.2	0.0	638.2	638.2	5.3	638.2
Vapor Fraction	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Mass Flow (lb/hr)	56573	56573	65616	65616	453124	387504	387504
Component Mass Flow (lb/hr)							
Benzene	-	-	65616	65616	452800	387180	387180
Phenol	-	-	-	-	1	1	1
Catechol	-	-	-	-	-	-	-
Benzoic Acid	-	-	-	-	-	-	-
Benzaldehyde	-	-	-	-	-	-	-
Water	-	-	-	-	281	281	281
Oxygen	13120	13120	-	-	7	7	7
Nitrogen	43453	43453	-	-	35	35	35
Molar Flow (lbmol/hr)	1961	1961	840	840	5814	4974	4974
Operating Volume Flow (cuft/hr)	780844	30162	1212	1217	8835	7597	7621


Section 200-Reactor
100B
100A
300A
300B
htm
htm
htm
htm
E-201
E-202
E-203
E-204
E-205
R-201A/B
R-202A/B
R-203A/B
R-204A/B
R-201A/B Stage 1 Reactor
E-203 Stage 1 Cooler
R-202A/B Stage 2 Reactor
E-204 Stage 2 Cooler
R-203A/B Stage 3 Reactor
R-204A/B Stage 4 Reactor
E-205 Stage 3 Cooler
E-202 Feed Pre-Heater
E-201 Feed/Effluent Exchange
2
5
6
7
8
9
10
11

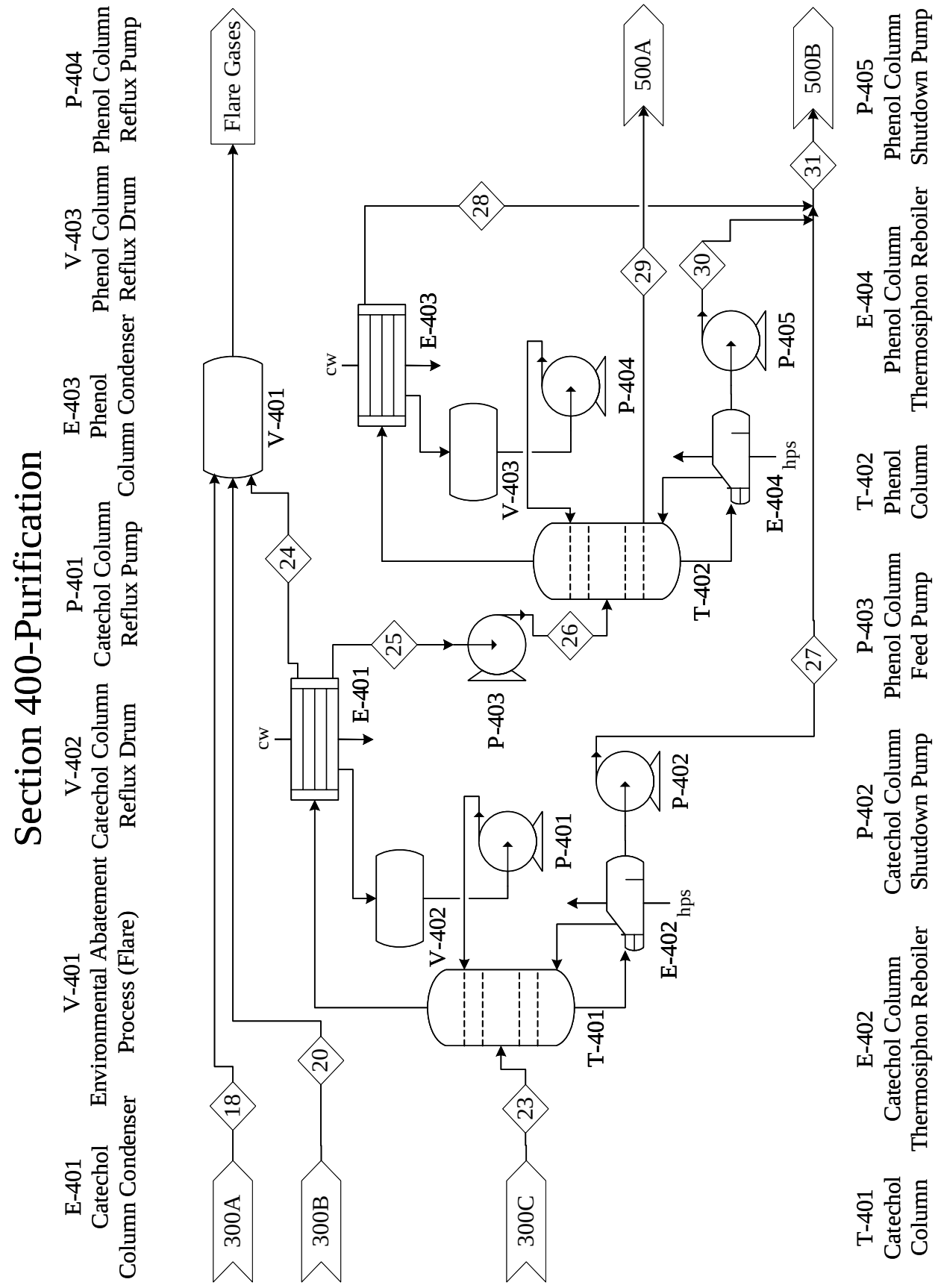
Stream Number	2	5	6	7	8	9	10
Temperature (°F)	384.1	165	515.4	698	665	662	441.5
Pressure (psig)	580.2	638.2	636.4	631.4	580.1	580.1	575.6
Vapor Fraction	1.0	0.0	0.0	1.0	1.0	1.0	1.0
Mass Flow (lb/hr)	56573	453124	453124	453124	509697	509697	190451
Component Mass Flow (lb/hr)							
Benzene	-	452800	452800	452800	452800	396200	139430
Phenol	-	1	1	1	1	66011	8743
Catechol	-	-	-	-	-	2234	147
Benzoic Acid	-	-	-	-	-	152	6
Benzaldehyde	-	-	-	-	-	132	16
Water	-	281	281	281	281	304	158
Oxygen	13120	7	7	7	13127	1176	1073
Nitrogen	43453	35	35	35	43488	43488	40878
Molar Flow (lbmol/hr)	1961	5814	5814	5814	7775	7402	3381
Operating Volume Flow (cuft/hr)	30162	8835	14402	85231	138890	127830	47368

Stream Number	11
Temperature (°F)	441.5
Pressure (psig)	575.6
Vapor Fraction	0.0
Mass Flow (lb/hr)	319246
Component Mass Flow (lb/hr)	
Benzene	256770
Phenol	57268
Catechol	2087
Benzoic Acid	146
Benzaldehyde	116
Water	146
Oxygen	103
Nitrogen	2610
Molar Flow (lbmol/hr)	4021
Operating Volume Flow (cuft/hr)	7892


Section 300-Separations
C-301 Vapor Effluent Turbine
E-301 Vapor Effluent Steam Formation
E-302 Vapor Effluent Cooler
V-301 Benzene Column Reflux Drum
T-301 Flash Drum
E-305 Benzene Column Condenser
P-301 Liquid Effluent Turbine
E-303 Liquid Effluent Steam Formation
E-304 Liquid Effluent Cooler
T-302 Benzene Column
P-302 Benzene Column Reflux Pump
E-304 Benzene Column Thermosiphon Reboiler
P-303 Benzene Column Shutdown Pump
200A
200B
400A
400B
100
400C
C-301
P-301
E-301
E-302
E-303
E-304
E-305
E-306
V-301
T-301
T-302
P-302
P-303
bfw
cw
hps
10
11
12
13
14
15
16
17
18
19
20
21
23

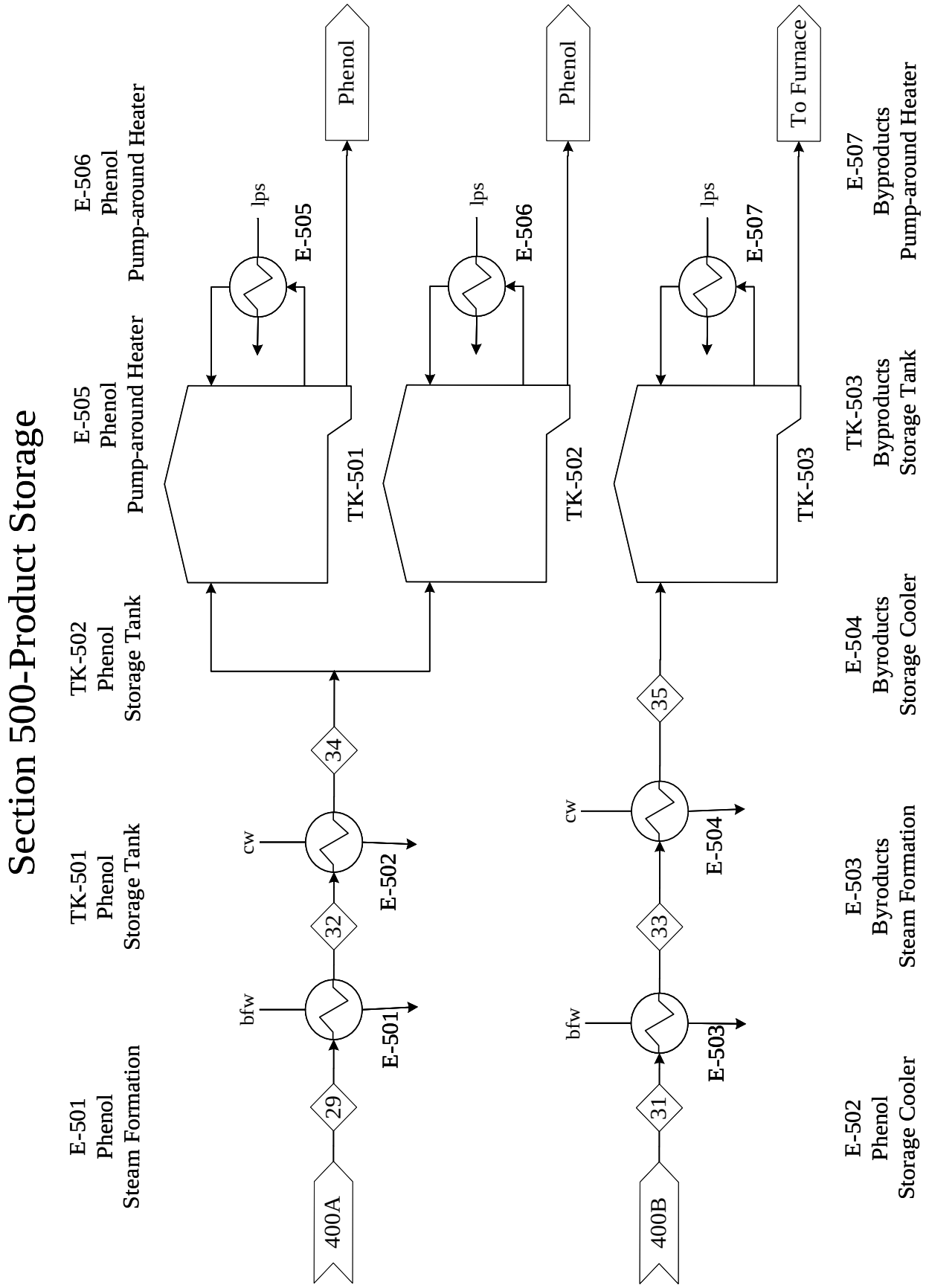
Stream Number	10	11	12	13	14	15	16
Temperature (°F)	441.5	441.5	327.5	437.0	285	285	110
Pressure (psig)	575.6	575.6	155.0	155.0	150.0	150.0	145.0
Vapor Fraction	1.0	0.0	0.97	0.0	0.75	0.03	0.45
Mass Flow (lb/hr)	190451	319246	190451	319246	190451	319246	190451
Component Mass Flow (lb/hr)							
Benzene	139430	256770	139430	256770	139430	256770	139430
Phenol	8743	57268	8742	57268	8743	57268	8743
Catechol	147	2087	147	2087	147	2087	147
Benzoic Acid	6	146	6	146	6	146	6
Benzaldehyde	16	116	16	116	16	116	16
Water	158	146	158	146	158	146	158
Oxygen	1073	103	1073	103	1073	103	1073
Nitrogen	40878	2610	40878	2610	40878	2610	40878
Molar Flow (lbmol/hr)	3381	4021	3381	4021	3381	4021	3381
Operating Volume Flow (cuft/hr)	47368	7892	152630	7838	118960	12243	60759

Stream Number	17	18	19	20	21	23
Temperature (°F)	110	110.1	110.1	172.4	172.4	389.8
Pressure (psig)	145.0	145.0	145.0	5.3	5.3	8.7
Vapor Fraction	0.02	1.0	0.0	1.0	0.0	0.0
Mass Flow (lb/hr)	319246	47014	462675	6369	387504	68803
Component Mass Flow (lb/hr)						
Benzene	256770	3233	392960	5498	387180	284
Phenol	57268	9	66002	-	1	66001
Catechol	2087	-	2234	-	-	2234
Benzoic Acid	146	-	152	-	-	152
Benzaldehyde	116	-	132	-	-	132
Water	146	8	296	14	281	-
Oxygen	103	1108	68	61	7	-
Nitrogen	2610	42656	831	796	35	-
Molar Flow (lbmol/hr)	4021	1599	5803	102	4974	728
Operating Volume Flow (cuft/hr)	8668	60919	8422	33696	7597	1201


Section 400-Purification
E-401 Catechol Column Condenser
V-401 Environmental Abatement Process (Flare)
V-402 Catechol Column Reflux Drum
P-401 Catechol Column Reflux Pump
E-403 Phenol Column Condenser
V-403 Phenol Column Reflux Drum
P-404 Phenol Column Reflux Pump
T-401 Catechol Column
E-402 Catechol Column Thermosiphon Reboiler
P-402 Catechol Column Shutdown Pump
P-403 Phenol Column Feed Pump
T-402 Phenol Column
E-404 Phenol Column Thermosiphon Reboiler
P-405 Phenol Column Shutdown Pump
300A
300B
300C
Flare Gases
500A
500B
cw
hps
18
20
23
24
25
26
27
28
29
30
31

Stream Number	18	20	23	24	25	26	27
Temperature (°F)	110.1	172.4	389.8	377.1	377.1	377.2	476.1
Pressure (psig)	145.0	5.3	8.7	5.3	5.3	15.3	8.8
Vapor Fraction	1.0	1.0	0.0	1.0	0.0	0.0	0.0
Mass Flow (lb/hr)	47014	6369	68803	656	65463	65463	2684
Component Mass Flow (lb/hr)							
Benzene	3233	5498	284	28	256	256	-
Phenol	9	-	66001	626	65076	65076	299
Catechol	-	-	2234	-	1	1	2233
Benzoic Acid	-	-	152	-	-	-	152
Benzaldehyde	-	-	132	2	130	130	-
Water	8	14	-	-	-	-	-
Oxygen	1108	61	-	-	-	-	-
Nitrogen	42656	796	-	-	-	-	-
Molar Flow (lbmol/hr)	1599	102	728	7	696	696	25
Operating Volume Flow (cuft/hr)	60919	33696	1201	3063	1139	1140	44

Stream Number	28	29	30	31
Temperature (°F)	303.6	394.6	395.6	374.4
Pressure (psig)	5.3	9.7	10.0	5.3
Vapor Fraction	0.0	1.0	0.0	0.08
Mass Flow (lb/hr)	2162	63256	44	4890
Component Mass Flow (lb/hr)				
Benzene	255	1	-	255
Phenol	1883	63148	44	2226
Catechol	-	1	-	2233
Benzoic Acid	-	-	-	152
Benzaldehyde	23.9	106	0.1	24
Water	-	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Molar Flow (lbmol/hr)	24	672	1	49
Operating Volume Flow (cuft/hr)	37	243690	1	1878


Section 500-Product Storage
E-501
Phenol
Steam Formation
TK-501
Phenol
Storage Tank
E-502
Phenol
Storage Cooler
TK-502
Phenol
Storage Tank
E-503
Byproducts
Steam Formation
E-504
Byproducts
Storage Cooler
TK-503
Byproducts
Storage Tank
E-505
Phenol
Pump-around Heater
E-506
Phenol
Pump-around Heater
E-507
Byproducts
Pump-around Heater
400A
400B
29
31
32
33
34
35
bfw
cw
lps
E-501
E-502
E-503
E-504
E-505
E-506
E-507
TK-501
TK-502
TK-503
Phenol
Phenol
To Furnace

Stream Number	29	31	32	33	34	35
Temperature (°F)	394.6	374.4	285	285	113	113
Pressure (psig)	9.7	5.3	4.7	0.0	0.0	0.0
Vapor Fraction	1.0	0.08	0.0	0.0	0.0	0.0
Mass Flow (lb/hr)	63256	4890	63256	4890	63256	4890
Component Mass Flow (lb/hr)						
Benzene	1	255	1	255	1	255
Phenol	63148	2226	63148	2226	63148	2226
Catechol	1	2233	1	2233	1	2233
Benzoic Acid	-	152	-	152	-	152
Benzaldehyde	106	24	106	24	106	24
Water	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-
Nitrogen	-	-	-	-	-	-
Molar Flow (lbmol/hr)	672	49	672	49	672	49
Operating Volume Flow (cuft/hr)	243690	1878	1040	77	954	71

Section 13

Process Descriptions

Section 13.1: Section 000-Feed Storage

A benzene storage tank is employed to hold one day's worth of feedstock. This was chosen to prevent against a complete production halt due to on site pipeline malfunctions, or to increase production on days with greater demand. Stream 3 feeds into the process at a rate of 65,616 lb/hr at ambient conditions. The specification sheet for the feed storage tank can be found in Section 16, pg. 103.

Section 13.2: Section 100- Feed

To account for pressure drops across heat exchangers and reactors, the fresh benzene is pumped above reaction pressure. Benzene recycled from the process is also pumped to this same pressure and then combined with the fresh feed. The two benzene sources are pumped separately to prevent any partial vaporization that would occur if the two streams were mixed prior to pressurization. The mixed stream proceeds to process section 200. Ambient air passes through the three-stage multi-stage air compressor at a rate of 56,573 lb/hr and is pressurized to reaction pressure. Intercoolers with cooling water are used here to ensure that extreme temperatures do not affect the structural stability of the equipment. The pressurized air is then passed to process section 200. Specification sheets for the pumps and compressor can be found in Section 16, pgs. 92-94.

Section 13.3: Section 200- Reactor

The mixed benzene in stream 5 is pre-heated using a counter-current heat exchanger which also slightly cools and partially condenses the vapor effluent leaving in stream 9. The cold outlet in stream 6 is then heated up to slightly above reaction conditions using heating oil. The benzene is then mixed with the cooler air and stream 8 is fed into the reactor at reaction conditions. Oxygen

concentration within the reactor is 2.6% by mass, which is below the maximum allowable level of 5% for explosion considerations. The process is designed to assume a realistic oxygen limiting reagent conversion of 91.4%.

For the purposes of simulation, the reaction is assumed to be carried out in a single packed bed reactor vessel at the isothermal and isobaric conditions described in the patent. In reality, we propose separating the reactor into four equivalent stages, each assumed to account for one fourth of the total benzene converted. A total adiabatic temperature rise, due to the highly exothermic reactions, was determined to be 216 °F. An allowable temperature rise per reactor unit was set at 54 °F, which would necessitate 4 reactor stages with 3 intercoolers. The flow in each packed bed section is designed to go from the bottom to the top. The reactor inlet would be fed at 27 °F below reaction conditions, allowed to raise the 54 °F, and would leave each reactor stage at 27 °F above reaction conditions. After each intermediate reactor stage, the effluent is cooled back down to feed conditions via heating oil (see Section 14.1, pg. 65). The ability of heating oil to withstand elevated temperatures without undergoing any phase change makes it the preferred heat transfer media for cooling the reactor. Cooling water used under these same conditions would likely form a steam envelope and greatly diminish the operational heat transfer coefficient. Reactor design allows for the average temperature across each reactor stage would be the isothermal reactor temperature given in the patent. A liquid hourly space velocity (LHSV) of 100 $\frac{mL\ benzene}{hr*g_{catalyst}}$ =1.60 $\frac{ft^3\ benzene}{hr*lb_{catalyst}}$ was chosen from the patent data (as discussed in Section 10.1, pg. 33), and catalyst volume, total reactor dimensions, and total pressure drop across the reactor were determined accordingly (see Section 15.1.3, pg. 76). The pressure of the feed streams would be slightly higher than reaction conditions,

such that the average pressure across the reactor vessel would be the isobaric reactor pressure given in the patent.

To preheat the reactor feed, exchanger E-201 is used to cool the reactor effluent by transferring 88,350,260 BTU/hr of thermal energy from the effluent to the feed. This cooling process partially condenses the effluent of this vapor phase reaction, requiring two nozzles at the outlet of the heat exchanger for the vapor and liquid effluent phases. These two separate phase effluent streams are then sent to section 300. Specification sheets for the effluent heat exchanger and reactor vessels can be found in Section 16, pgs. 97-98.

Section 13.4: Section 300- Separations

Based on thermodynamic results from ASPEN, operating conditions of 110.1 °F and 145 psig were chosen for the flash drum to maximize off-gassing of the non-condensable oxygen and nitrogen at 98%, while also minimizing benzene loss to 0.8%. Turbines are employed to help lower the pressure of streams 10 and 11 to flash conditions and recover useful work in the form of 2239 kWh of electricity (see Section 14.1, pg. 65). Each effluent stream is then cooled with boiler feed water to a temperature of 285 °F to produce a total of 40,772 lb/hr low pressure 15 psig saturated steam for use in section 500 of the process. Excess low pressure steam produced will be sold elsewhere within the plant complex (see Section 15, pg. 50, Section 14.1, pg. 65, Section 19, pg. 119). A temperature approach of 35 °F was used to ensure the occurrence of nucleate boiling. Streams 14 and 15 are then cooled the remainder of the way using cooling water. The flash vapor is collected in a flare hood and sent to section 400 for environmental abatement procedures. Design of the flash drum can be found in Section 15.1.4, pg.78.

After off-gassing, the liquid exit from T-301 is fed to the first distillation column, T-302, whose main purpose is to separate the benzene and remaining non-condensables from phenol and the other organic byproducts. Design of distillation column 1 can be found in Section 15.1.4, pg.79. Operating at a condenser pressure of 5.3 psig, the column uses 32 trays to separate the remaining non-condensables from the bottoms stream 23. The partial condenser, with a distillate vapor fraction of 0.02, produces one vapor and one liquid distillate stream at 172.4 °F using cooling water. The liquid distillate in stream 21 is then fed back around to section 100 to act as the process benzene recycle stream. This column was optimized to reach a benzene recycle of 97.7% of the total unreacted benzene leaving the reactor in stream 9. A thermosiphon reboiler uses high pressure steam to maintain a temperature of 389.8 °F. The vapor distillate and the bottoms product continue on to process section 400. A shutdown pump, P-303, is included for shutdown operations, to aid the transfer of remaining liquid to the next process section in the absence of normal fluid pressure. Specification sheets for the two turbines, flash drum, and distillation column can be found in Section 16, pgs. 95-96, 99-100.

Section 13.5: Section 400- Purification

The bottoms product from the first column is sent to distillation column 2 to separate out the heavy byproducts, which are represented in our simulation as catechol and benzoic acid. Distillation column 2 was designed much more rigorously than would be necessary in practice, due to the similar chemical structures of phenol and catechol. Other potential heavy products would likely be even heavier and thus more easily removed. The methods used to design distillation column 2 can be found in Section 15.1.4, pg. 81. Operating at a condenser pressure of 5.3 psig, the column uses 20 trays to separate phenol and benzaldehyde from benzoic acid and

catechol. The partial condenser, with a distillate vapor fraction of 0.01, aids in the slight removal of some of the benzaldehyde and produces two distillate streams at 377.1 °F using cooling water. This column was optimized to remove 99.98% of the catechol and 100% of the benzoic acid. A thermosiphon reboiler uses high pressure steam to maintain a temperature of 476.1 °F. The vapor distillate is taken off and combined in a collection hood with the vapor exit from T-301 and vapor distillate from T-302. These vapors are then sent to a flare system. Based on consultant recommendations, approximately 10,000,000 BTU/hr of natural gas are used to fuel an auto-oxidation reaction to safely dispose of environmentally hazardous compounds. A shutdown pump, P-402, is included for shutdown operations, to aid the transfer of remaining liquid to the next distillation column in the absence of normal fluid pressure.

The liquid distillate in stream 25 is pumped into the lower half of distillation column 3 at stage 16. The purpose of distillation column 3 is to perform the most rigorous separation of the entire process between phenol and benzaldehyde, which are extremely close boilers within 7 °F of each other at the column pressure of 10 psig. The methods for designing distillation column 3 can be found in Section 15.1.4, pg. 83. Since phenol is the heavier component, we proposed pulling the phenolic product off as a vapor at stage 20, which ensures the greatest purity. This also accounts for the possibility of further removal of any other heavy products that weren't removed in column 2. Since benzaldehyde serves as a placeholder chemical for a category of potential byproducts and is a much closer boiler to phenol than any real potential byproduct, we assert that our purification system is more than sufficient to attain a desired purity of 99.8% phenol by mass. Using our placeholder chemicals, the product purity in stream 29 was optimized to be 99.83% phenol by mass. Operating at a condenser pressure of 5.3 psig, the column uses 22 trays to separate phenol from remaining organic impurities. A total condenser, used here at 303.6 °F with cooling water, is

an allowable simplification since all non-condensables should have been previously removed from the process. A thermosiphon reboiler uses high pressure steam to maintain a temperature of 395.6 °F. A shutdown pump, P-405, is included for shutdown operations. The bottoms products of the two distillation columns are combined with the liquid distillate of column 3, and sent to section 500 to be stored for use as furnace fuel to help offset the need for natural gas. The desired product stream 29 is also sent to the next process section for storage. Specification sheets for the two distillation columns can be found in Section 16, pgs. 101-102.

Section 13.6: Section 500- Product Storage

As was the case with the two effluent streams in section 300, the two streams 29 and 31 sent to the storage section are cooled with boiler feed water to a temperature of 285 °F to produce a total of 17,873 lb/hr low pressure 15 psig saturated steam for use in this storage section and the excess to be sold (Section 14.1, pg. 65, Section 19, pg. 119). A temperature approach of 35 °F was used to ensure the occurrence of nucleate boiling. Streams 32 and 33 are then cooled the remainder of the way using cooling water. These insulated storage tanks are maintained at 113 °F and just above ambient pressure to ensure that the phenol product does not crystallize, as it would at ambient temperature. Each phenol storage tank is designed to hold up to one week's worth of product to account for variability in demand on-site and for distributors. This storage system also helps to account for variability in production while still maintaining enough product for the demand (see Section 15.1.5, pg. 86). The byproducts storage tank is designed to hold up to one day's worth of byproducts to allow for variability in natural gas availability, as well as to ensure that there is enough byproduct fuel to burn because of the relatively low flowrate of stream 35 (see Section 15.1.5, pg. 87). The pump-around flow of each phenol tank is 20,226 lb/hr to combat the

155,166 BTU/hr of heat lost through the insulation. The pump-around flow of the byproduct tank is 965 lb/hr to combat the 7,496 BTU/hr of heat lost through the insulation. The hourly flowrate of stream 34 of 63,256 lb/hr corresponds to 500,987,520 lb/operating-year which meets the process design criteria. Specification sheets for the storage tanks can be found in Section 16, pgs. 104-105.

Section 14

Energy Balance & Utility Requirements

Section 14.1: Heat Integration Strategy

Heat integration was a significant focus of our design in the hopes of minimizing lost heat and work, which consequently minimizes utility costs. A summary of the main heat integrations can be found in Table 14.1 below. The primary technique employed was evaluating the presence of high temperature streams that needed to be cooled, and using them to either produce steam or pre-heat other streams. This is most apparent when the reactor effluent in stream 9 is used to pre-heat the reactor feed in stream 5 via counter-current heat exchanger (see Section 12, pg. 48 and Section 15.1.2, pg.74).

To heat stream 6 to 698 °F, slightly above reactor conditions, heating oil is employed as a heat transfer media. Instead of using a furnace to heat the oil to the necessary conditions from ambient conditions for each iteration through its internal heat transfer loop, we elected to use the oil as a cooling fluid for the reactor intercoolers. This allows us to cool the reactor with a fluid that is capable of withstanding high reaction temperatures, while simultaneously recovering additional energy from the reaction stream. The furnace duty on H-001 would have been 77,555,400 BTU/hr (duty on E-202) for each pass through the oil heating loop. This value is effectively reduced by 44,778,808 BTU/hr (or 14,926,269 BTU/hr per reactor intercooler) to be 32,776,592 BTU/hr. This reduced furnace duty is the total amount of energy required to heat the oil from its temperature after cooling the reactors of 654 °F to its maximum temperature within its heat loop of 705 °F. The mass flow of heating oil is assumed to remain constant at 1,000,000 lb/hr and is continuously recycled throughout the heat transfer loop from a minimum temperature of 585 °F to a maximum temperature of 705 °F through the reactor intercoolers to furnace to reactor feed heater.

The utility of the heating oil furnace would normally come from enough natural gas to achieve the required duty. However, we offset the amount of natural gas fuel required by reusing

our organic byproducts from stream 35 and stored in TK-503 as additional fuel. This reduces the heat duty needed from burning the natural gas by 4,636,836 BTU/hr to a final required heat duty of 28,139,756 BTU/hr from natural gas fuel.

While 88,350,260 BTU/hr of energy used to achieve the high reaction temperature are recovered with the effluent heat exchanger E-201, we attempt to recover even more. During the cooling of the effluent streams 10 and 11 down to flash conditions, we use E-301 and E-303 to produce a total of 40,722 lb/hr low pressure 15 psig steam. The same thing is done when cooling the hot products of streams 29 and 31 from distillation column 3 down to storage conditions. Here, E-501 and E-503 are used to produce a total of 17,873 lb/hr low pressure 15 psig steam. Since the total amount of low pressure steam required for the heated storage tanks is 336 lb/hr, the remaining 58,309 lb/hr 15 psig steam produced is taken to be sold, presumably to other locations within the plant site. See Section 15, pg. 86 for storage tank designs.

Due to the high reaction pressure, we are also able to produce electricity from two turbines: a gas expander on the vapor effluent stream 10, and a liquid expander on the liquid effluent stream 11. The pressure drop from 575.6 psig to 155.0 psig allows us to recover a net of 2239 kWh, which we then use to partially power the multistage air compressor C-101-3. This reduces the net electrical requirement for the compressor from 3451 kWh to 1212 kWh.

Table 14.1. Summary of heat and electrical integrations with clear paths to satisfaction from demand. The associated textboxes explain the source of the heat and electricity to be integrated for the indicated demand.

Heating or Electrical Process	**Heat Duty (BTU/hr)**	**ΔT (°F)**
Feed to Reactor (Stream 5 to 7)	165,905,660	165 → 698
Heating Oil Loop	77,555,400	585 → 705
Phenol Storage	155,166 per tank	86 → 113
Byproduct Storage	7495	86 → 113
Air Compressor	3451 kWh	-

a) 88,350,260 BTU/hr as Stream 9 is cooled from 662 °F to 441.5 °F
b) 77,555,400 BTU/hr from heating oil

a) 14,926,269 BTU/hr from each reactor intercooler as the intermediate effluent is cooled from 693 °F to 635 °F
b) 32,776,592 BTU/hr from the furnace H-001

a) 155,166 BTU/hr from 164 lb/hr 15 psig steam produced from E-301, E-303, E-501, or E-503

a) 7495 BTU/hr from 8 lb/hr 15 psig steam produced from E-301, E-303, E-501, or E-503

a) 2239 kWh from turbines on Streams 10 and 11
b) 1212 kWh via purchased electricity

Section 14.2: Process Utilities

Table 14.2 summarizes the annual utilities and electricity needed for each process unit per hour and per operating year (op-yr). The net utility requirements, accounting for heat integration strategies, is also included. Table 14.3 indicates the total utility requirements per pound phenol produced. The density of cooling water and boiler feed water was taken at 8.33 lb/gal.

Table 14.2. Net utility requirements per hour and per operating year by process unit and utility type.

Utility	**Equipment Item**	**Quantity (per hr)**	**Quantity (per op-yr)**
Cooling Water (lb)	E-101	195,287	1.55×10^9
	E-102	234,875	1.86×10^9
	E-302	1,379,310	1.09×10^{10}
	E-304	1,390,817	1.10×10^{10}
	E-305	5,743,677	4.55×10^{10}
	E-401	3,877,717	3.07×10^{10}
	E-403	860,802	6.82×10^9
	E-502	279,640	2.21×10^9
	E-504	21,811	1.73×10^8
	Total (lb)	***13,983,937***	***1.11×10^{11}***
High Pressure Steam (500 psig) (lb)	E-306	163,029	1.29×10^9
	E-402	92,560	7.33×10^8
	E-404	38,568	3.05×10^8
	Total (lb)	***294,186***	***2.33×10^9***
Low Pressure Steam (15 psig) (lb)	E-505	164	1.30×10^6
	E-506	164	1.30×10^6
	E-507	8	6.28×10^4
	Subtotal	***336***	***2.66×10^6***
	Steam Produced	***(58,645)***	***(4.64×10^8)***
	Net Utility (lb)	***(58,309)***	***(4.62×10^8)***
Boiler Feed Water (lb)	E-301	12,291	9.73×10^7
	E-303	28,481	2.26×10^8
	E-501	17,565	1.39×10^8
	E-503	308	2.44×10^6
	Total (lb)	***58,645***	***4.64×10^8***
Electricity (kWh)	C-101-3	3451	2.73×10^7
	P-101	72	5.66×10^5
	P-102	340	2.69×10^6
	P-302	9	6.79×10^4
	P-303	3	2.56×10^1
	P-401	10	7.85×10^4
	P-402	2	1.39×10^1
	P-403	1	8.44×10^3
	P-404	3	2.43×10^4
	P-405	1	7.27×10^0
	Subtotal	***3892***	***3.08×10^7***
	Electricity Produced	***(2239)***	***(1.77×10^7)***
	Net Utility (kWh)	***1653***	***1.30×10^7***
Natural Gas Fuel (BTU)	H-001	32,776,592	2.60×10^{11}
	V-401	10,000,000	7.92×10^{10}
	Subtotal	***42,776,592***	***3.39×10^{11}***
	Byproduct Fuel	***(4,636,836)***	***(3.67×10^{10})***
	Net Utility (BTU)	***38,139,756***	***3.02×10^{11}***

Table 14.3 Total utility requirements per lb phenol produced.

Utility	**Unit**	**Ratio (per lb phenol)**
Cooling Water	lb	221.07
High Pressure Steam	lb	4.65
Low Pressure Steam	lb	(0.92)
Boiler Feed Water	lb	0.93
Electricity	kWh	0.03
Natural Gas Fuel	BTU	602.94

Section 15

Equipment List and Unit Descriptions

The following section is divided into two sections. The first section discusses major process equipment units with specification sheets found in section 16. The second section details minor process equipment composed of mostly process heaters whose unit size was estimated with simplified correlations from *Seider et. al, 2017.*

Section 15.1: Major Process Units

Section 15.1.1: Pumps, Compressors, and Turbines

Air Compressor

Unit ID: C-101-3

Type: Multi-stage Compressor

Material: Cast Iron

Specification Sheet: Section 16, pg. 92

Costing data: Section 17.1.1, pg. 109

Temperature: 384.1 °F

Pressure: 580.2 psig

Work: 4629 hp

The multi-stage air compressor was designed with the aid of ASPEN to achieve a compression ratio of about 2-3 per stage, resulting in a 3-stage compressor. To avoid melting the compressor, a temperature of 100 °F was set for the beginning of each stage, which resulted in 2 intercoolers removing 3,151,165 BTU/hr and 4,227,753 BTU/hr using 195,287 lb/hr and 234,875 lb/hr of cooling water respectively. A pressure drop of 5 psi was assumed for the intercoolers. An approximate isentropic efficiency for each stage was taken to be 0.85. Cast iron was chosen since it is the cheapest option and will not react with air.

Feed Pump

Unit ID: P-101 Temperature: 92.1 °F

Type: Pump Pressure: 638.2 psig

Material: Cast Iron Work: 95.6 hp

Specification Sheet: Section 16, pg. 93

Costing data: Section 17.1.1, pg. 109

The feed pump was designed with the aid of ASPEN to maintain a flow of 1217 ft^3/hr by using 71.4 kWh of electricity. A head of 1698 ft was calculated based on Appendix 4.1, pg. 212. Guidelines[15.1] suggest a centrifugal pump in Horizontal Split Case (HSC) orientation with 2 stages, shaft rpm of 3600, and a maximum motor hp of 1450. Cast iron was chosen since it is the cheapest option and will not react with benzene.

Recycle Pump

Unit ID: P-102 Temperature: 176.6 °F

Type: Pump Pressure: 638.2 psig

Material: 316 Stainless Steel Work: 457 hp

Specification Sheet: Section 16, pg. 94

Costing data: Section 17.1.1, pg. 109

The recycle pump was designed with the aid of ASPEN to maintain a flow of 7621 ft^3/hr by using 340.2 kWh of electricity. A head of 1787 ft was calculated based on Appendix 4.1, pg.

[15.1] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.452.

212. Guidelines[15.2] suggest a centrifugal pump in Horizontal Split Case (HSC) orientation with 2 stages, shaft rpm of 3600, and a maximum motor hp of 1450. Due to the possibility of benzoic acid and other corrosive byproducts being present in the recycle, a construction material of 316 stainless steel was chosen.

Vapor Effluent Turbine

Unit ID: C-301 Temperature: 441.5 °F

Type: Gas Expanding- Compression Design Turbine Pressure: 155.0 psig

Material: 316 Stainless Steel Work: -2858 hp

Specification Sheet: Section 16, pg. 95

Costing data: Section 17.1.1, pg. 109

The vapor effluent turbine was designed with the aid of ASPEN to reduce the pressure of stream 10 and maintain a flow of 152,630 ft^3/hr. Guidelines[15.3] suggest an approximate isentropic efficiency of 0.85 and mechanical efficiency of 0.98. Due to the presence of benzoic acid and other corrosive byproducts, a construction material of 316 stainless steel was chosen.

[15.2] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.452.
[15.3] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.473.

Liquid Effluent Turbine

Unit ID: P-301 Temperature: 441.5 °F

Type: Liquid Expanding- Centrifugal Pump Design Pressure: 155.0 psig

Material: 316 Stainless Steel Work: -145 hp

Specification Sheet: Section 19, pg. 96

Costing data: Section 17.1.1, pg. 109

The liquid effluent turbine was designed with the aid of ASPEN to reduce the pressure of stream 11 and maintain a flow of 7838 ft^3/hr. Guidelines[15.4] suggest an approximate isentropic efficiency of 0.6. Due to the presence of benzoic acid and other corrosive byproducts, a construction material of 316 stainless steel was chosen.

Section 15.1.2: Process Heat Exchangers

Effluent Heat Exchanger

Unit ID: E-201 Temperature: 662 °F

Type: Counter-current Heat Exchanger Pressure: 638.2 psig

Material: 316 Stainless Steel Area: 8401.5 ft^2

Heat Exchanged: 88,350,260 BTU/hr

Specification Sheet: Section 19, pg. 97

Costing data: Section 17.1.2, pg. 109

With the aid of ASPEN Exchanger Design and Rating (EDR), the counter-current shell-and-tube effluent heat exchanger was designed in accordance with Tubular Exchanger

[15.4] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.473.

Manufacturers Association (TEMA) standards. Unit E-201 was optimized for our process to cool the reactor effluent and harness that thermal energy to pre-heat the reactor feed. This design also limits the exchanger to a single unit with no additional shells in series or parallel (See TEMA sheet in Appendix 4.2.2, pg. 215). All design values and calculations were taken directly from ASPEN. This one shell/unit design allows for a smaller exchanger and lower purchasing costs. Horizontal type DEU was selected. Type D accounts for a high pressure shell. Since the hot fluid partially condenses upon cooling (necessitating the need of two outlet nozzles), the hot fluid is set to the tube side, and type E is used for a single phase cold fluid on the shell side. A U-tube head is used as the least expensive type which also accounts for the possibility of thermal expansion of the material. The number of tube passes was set to 2 as the minimum allowable number for a U-tube exchanger. A 30 inch triangular tube pattern was used as the most compact design. We suggest the use of a single segmental baffle as the most common type since we assume our fluids are non-fouling. However, a low value fouling factor was included as a safety factor. A construction material for both the tubes and the shell was chosen as 316 stainless steel since it can handle the high temperatures and prevent against potential deterioration from corrosive byproducts. This design lead to a total number of tubes of 700 with outer diameters of 0.75 in, length of 360 in, and pitch of 0.9375 in. The shell was also found to have an outer diameter of 42.2047 in, with a service (practical dirty) heat transfer coefficient of 85.67 BTU/(hr-ft^2-°F) and log-mean-temperature-difference (LMTD) of 122.76 °F.

Section 15.1.3: Reactors

Reactor Vessels

Unit ID: R-201-4A/B Temperature: 662 °F

Type: Reactor Pressure: 580.1 psig

Material: Carbon Steel Outer Shell Height: 9.12 ft/unit

316 Stainless Steel Inner Lining Diameter: 9.12 ft

Heat Removed per Intercooler: 14,926,269 BTU/hr

Specification Sheet: Section 16, pg. 98

Costing data: Section 17.1.3, pg. 110

The following describes the equations found in Appendix 4.3, pg. 216. As previously discussed in Section 13.3, pg. 57, the allowable temperature rise, based on the total adiabatic temperature rise of the exothermic reaction, led to a design of 4 vertical reactor sections with 3 intercoolers. The flow in each packed bed section was designed to go from the bottom to the top. A critical assumption is made that one-fourth of the reaction occurs equivalently in each of the four stages. All catalyst properties were taken to be that of bulk alumina (ρ=40.02 lb/ft^3) with a lifetime of 6 months. It was also assumed that the catalyst cannot be regenerated, and would require replacement at the end of its lifetime. Guidelines[15.5] suggest an approximate catalyst particle diameter of 0.016 ft and bed porosity of 0.42 for porous solids. To conserve space, an L/D aspect ratio for the overall vertical reactor was set to 4. An LHSV of 100 $\frac{mL\ benzene}{hr*g_{catalyst}}$ =1.60 $\frac{ft^3\ benzene}{hr*lb_{catalyst}}$ was chosen based on the patent (as discussed in Section 10.3, pg. 38). In conjunction with the total volumetric flowrate passing through the reactor, the LHSV was used to calculate a total mass of

[15.5] Bartholomew, C.H., and R.J. Farrauto, "Fundamentals of Industrial Catalytic Processes, Second Edition", John Wiley & Sons Inc., 2006, pg.81.

catalyst of 86,707 lb, or 21,677 lb per section. The assumed catalyst bulk density led to a total catalyst volume of 2167 ft^3. Accounting for a 10% safety factor in reactor volume, and assuming that the volume of the bulk catalyst is equivalent to the volume of the packed bed, the total reactor volume was calculated to be 2384 ft^3. The volumetric flow of 138,890 ft^3/hr of the feed led to a total reactor residence time of 1.03 minutes, or 15.4 seconds per reactor section. The aspect ratio of 4 was used to determine the reactor diameter and overall reactor length. To separate the reactor into 4 sections, the diameter was held constant and the length divided by 4. Therefore, each reactor section has an L/D ratio of 1. The reactor has an overall diameter of 9.12 ft, length of 36.5 ft, and length per reactor unit of 9.12 ft. Reactor diameter was designed to be below 18 ft for ease of transport. The Ergun equation was then used to find the total packed bed pressure drop and pressure drop per bed section. A reasonable pressure drop across each reactor section was determined to be 2.14 psi, which amounted to a total pressure drop of 8.55 psi across all sections of the packed bed reactor.

As mentioned in Section 14.1, pg. 65, each intercooler removes 14,926,269 BTU/hr via 1,000,000 lb/hr of heat transfer media heating oil in exchangers with areas of 4429, 2076, and 8621 ft^2, each with a heat transfer coefficient estimated[15.6] as 30 BTU/hr/ft^2/°F.

To reduce costs, the reactor vessel was constructed out of a carbon steel outer shell, with a 1/8 in thick inner 316 stainless steel lining. The stainless steel is necessary to resist high temperatures and prevent against potential deterioration from corrosive byproducts. A fifth spare reactor vessel section will be purchased and swung into the process when any reactor section needs

[15.6] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

to be cleaned or have catalyst replaced. This swinging design would allow for easy reactor exchange with less downtime.

Section 15.1.4: Distillation Columns and Flash Drum

Flash Drum

Unit ID: T-301 Temperature: 110.1 °F

Type: Flash Drum Pressure: 145 psig

Material: Carbon Steel Outer Shell Functional Height: 25.2 ft

316 Stainless Steel Inner Lining Diameter: 8.4 ft

Specification Sheet: Section 16, pg. 99

Costing data: Section 17.1.4, pg. 110

The flash drum was optimized to off-gas 98% of the non-condensable oxygen and nitrogen, while also minimizing benzene loss to 0.8%. To size the flash drum according to the equations in Appendix 4.4, pg. 218, the total vapor fraction of the combined streams 16 and 17 was first determined to be 0.093. Based on common technique[15.7], our horizontal drum was designed with an L/D ratio of 3, a hold-up time of 5 min, a fraction of horizontal drum full of 0.5, and a vapor velocity design K-factor of 0.27 used to account for the vapor space in the drum. Correspondingly, the total volume of liquid held was then used to the find the design diameter of 8.4 ft and length of 25.2 ft. To reduce costs, the flash vessel was constructed out of a carbon steel outer shell, with a 1/8 in thick inner 316 stainless steel lining. The stainless steel was necessary to prevent against potential deterioration from corrosive byproducts.

[15.7] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.

Distillation Column 1

Unit ID: T-302	Temperature: 389.8 °F
Type: Distillation Column	Pressure: 8.7 psig
Material: Carbon Steel Outer Shell	Functional Height: 48 ft
316 Stainless Steel Inner Lining	Enriching Diameter: 15.5 ft
Specification Sheet: Section 16, pg. 100	Stripping Diameter: 17.5 ft
Costing data: Section 17.1.4, pg. 110	

With the aid of ASPEN, distillation column 1 was optimized to separate the unreacted benzene from the product phenol, and recycle up to 97.7% of the total amount of unreacted benzene from the reactor effluent. This required 12 theoretical stages, condenser pressure of 5.3 psig with an internal 2 psi pressure drop and subsequent 0.15 psi pressure drop per stage, a molar reflux ratio of 0.50 and molar bottoms rate of 728 lbmol/hr. Based on common technique[15.8], sieve trays were used with 4 passes per tray, and tray spacing of 1.5 ft. This produced hydraulic data with an enriching section diameter of 15.5 ft and stripping section diameter of 17.5 ft. We therefore propose that distillation column 1 be fabricated in two distinct halves, with a gradual slope joining the two. O'Connell correlations[15.9] (as described in Appendix 4.5, pg. 219) accounted for tray efficiencies and were used to calculate the total number of real trays at 32, with the feed tray located at 14, and an average tray efficiency of 0.32. The total number of real trays multiplied by the assumed tray spacing yielded a functional height of 48 ft, with an additional skirt length of 7 ft for the enriching section, and 10 ft for the stripping section.

[15.8] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.
[15.9] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.

Using a residence time of 5 minutes and L/D ratio of 2, the dimensions of the reflux accumulator modeled as a horizontal pressure vessel were determined with the equations found in Appendix 4.5, pg. 219 to be 7.44 ft diameter and 14.87 ft length. The head and electrical utility of the reflux pump set with a 25 psi pressure drop was determined to be 70.6 ft and 8.6 kWh respectively, with an isentropic efficiency of 0.71 from equations found in Appendix 4.1, pg. 212.

A partial condenser temperature of 172 °F and molar vapor fraction of 0.02 will be maintained with 2,671,478 lb/hr of cooling water in a 18,828 ft^2 exchanger with a heat transfer coefficient estimated[15.10] to be 60 BTU/hr/ft^2/°F. A thermosiphon reboiler is used for its efficient implementation of internal baffles, and will be maintained at a temperature of 390 °F with 163,029 lb/hr 500 psig high pressure steam in a 4496 ft^2 exchanger with a heat transfer coefficient estimated[15.11] to be 250 BTU/hr/ft^2/°F.

To reduce costs, the distillation column and reflux accumulator were each constructed out of a carbon steel outer shell, with a 1/8 in thick inner 316 stainless steel lining. The reflux pump, condenser, and reboiler were constructed solely out of the 316 stainless steel. A shutdown pump, P-303, was also included to account for pumping the remaining liquid in the bottom of the column through to the next process section during a plant shutdown. With an assumed height equal to 6 ft of liquid remaining at the bottom of the column, the pump was designed to operate for 15 minute blocks once every shutdown, which was assumed to be once a day for 35 days out of the year. This pump is capable of producing a head of 62.9 ft, electrical utility of 2.9 kWh, and was also constructed of 316 stainless steel.

[15.10] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, “Product and Process Design Principles”, John Wiley & Sons Inc., New Jersey, 2017, pg.376.
[15.11] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, “Product and Process Design Principles”, John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Distillation Column 2

Unit ID: T-401 Temperature: 476.1 °F

Type: Distillation Column Pressure: 8.8 psig

Material: Carbon Steel Outer Shell Functional Height: 30 ft

316 Stainless Steel Inner Lining Diameter: 12 ft

Specification Sheet: Section 16, pg. 101

Costing data: Section 17.1.4, pg. 110

With the aid of ASPEN, distillation column 2 was optimized to separate the unwanted heavier catechol byproduct from the product phenol, at a removal rate of up to 99.98% of the catechol from the phenol product. This required 12 theoretical stages, condenser pressure of 5.3 psig with an internal 2 psi pressure drop and subsequent 0.15 psi pressure drop per stage, a molar reflux ratio of 4.0 and molar distillate rate of 703 lbmol/hr. Based on common technique[15.12], sieve trays were used with 4 passes per tray, and tray spacing of 1.5 ft. This produced hydraulic data with an inside diameter of 12 ft. O'Connell correlations[15.13] (as described in Appendix 4.5, pg. 219) accounted for tray efficiencies and were used to calculate the total number of real trays at 20, with the feed tray located at 8, and an average tray efficiency of 0.53. The total number of real trays multiplied by the assumed tray spacing yielded a functional height of 30 ft, with an additional skirt length of 7 ft for the enriching section, and 10 ft for the stripping section.

Using a residence time of 5 minutes and L/D ratio of 2, the dimensions of the reflux accumulator modeled as a horizontal pressure vessel were determined with the equations found in

[15.12] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.
[15.13] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.

Appendix 4.5, pg. 219 to be 7.88 ft diameter and 15.75 ft length. The head and electrical utility of the reflux pump set with a 25 psi pressure drop was determined to be 62.7 ft and 9.9 kWh respectively, with an isentropic efficiency of 0.73 from equations found in Appendix 4.1, pg. 212.

A partial condenser temperature of 377 °F and molar vapor fraction of 0.01 will be maintained with 1,803,589 lb/hr of cooling water in a 4053 ft^2 exchanger with a heat transfer coefficient estimated[15.14] to be 60 BTU/hr/ft^2/°F. A thermosiphon reboiler is used for its efficient implementation of internal baffles, and will be maintained at a temperature of 476 °F with 92,590 lb/hr 500 psig high pressure steam in a 8498 ft^2 exchanger with a heat transfer coefficient estimated[15.15] to be 250 BTU/hr/ft^2/°F.

To reduce costs, the distillation column and reflux accumulator were each constructed out of a carbon steel outer shell, with a 1/8 in thick inner 316 stainless steel lining. The reflux pump, condenser, and reboiler were constructed solely out of the 316 stainless steel. A shutdown pump, P-402, was also included to account for pumping the remaining liquid in the bottom of the column through to the next process section during a plant shutdown. With an assumed height equal to 6 ft of liquid remaining at the bottom of the column, the pump was designed to operate for 15 minute blocks once every shutdown, which was assumed to be once a day for 35 days out of the year. This pump is capable of producing a head of 58.3 ft, electrical utility of 1.6 kWh, and was also constructed of 316 stainless steel.

[15.14] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.
[15.15] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Distillation Column 3

Unit ID: T-402	Temperature: 395.6 °F
Type: Distillation Column	Pressure: 10.0 psig
Material: Carbon Steel Outer Shell	Functional Height: 50 ft
316 Stainless Steel Inner Lining	Enriching Diameter: 5.5 ft
Specification Sheet: Section 19, pg. 102	Stripping Diameter: 7.5 ft
Costing data: Section 17.1.4, pg. 110	

With the aid of ASPEN, distillation column 3 was optimized to separate the close boiling benzaldehyde from the product phenol. Although responsible for the most rigorous separation, T-402 is the smallest distillation column in the process due to its position far downstream. It handles the lowest total mass and volumetric flowrates of material amongst all distillation columns. A product purity of 99.83% phenol by mass was achieved by pulling the phenol off as a side product vapor. This required 20 theoretical stages, condenser pressure of 5.3 psig with an internal 2 psi pressure drop and subsequent 0.15 psi pressure drop per stage, a molar reflux ratio of 29.25, molar distillate rate of 23.5 lbmol/hr, and molar side product vapor rate of 672 lbmol/hr. Based on common technique[15.16], sieve trays were used with 4 passes per tray, and tray spacing of 1.5 ft. This produced hydraulic data with an enriching section diameter of 5.5 ft and stripping section diameter of 7.5 ft. We therefore propose that distillation column 3 be fabricated in two distinct halves, with a gradual slope joining the two. O'Connell correlations[15.17] (as described in Appendix 4.5, pg. 219) accounted for tray efficiencies to calculate the total number of real trays at 22, with

[15.16] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.
[15.17] Kister, H.Z., P.M. Mathias, D.E. Steinmeyer, W.R. Penney, B.B. Crocker and J.R. Fair, "Equipment for Distillation, Gas Absorption, Phase Dispersion, and Phase Separation", 2008.

the feed tray located at 16, side product tray located at 20, and an average tray efficiency of 0.82. The total number of trays multiplied by the assumed tray spacing yielded a functional height of 50 ft, with an additional skirt length of 7 ft for the enriching section, and 10 ft for the stripping section.

Using a residence time of 5 minutes and L/D ratio of 2, the dimensions of the reflux accumulator modeled as a horizontal pressure vessel were determined with the equations found in Appendix 4.5, pg. 219 to be 4.87 ft diameter and 9.73 ft length. The head and electrical utility of the reflux pump set with a 25 psi pressure drop was determined to be 61.9 ft and 3.1 kWh respectively, with an isentropic efficiency of 0.57 from equations found in Appendix 4.1, pg. 212. The feed pump P-403 set with a 25 psi pressure drop has a head of 25.1 ft and electrical utility of 1.1 kWh.

A total condenser temperature of 304 °F will be maintained with 400,373 lb/hr of cooling water in a 1066 ft^2 exchanger with a heat transfer coefficient estimated[15.18] to be 60 BTU/hr/ft^2/°F. A thermosiphon reboiler is used for its efficient implementation of internal baffles, and will maintained at a temperature of 396 °F with 38,568 lb/hr 500 psig high pressure steam in a 4496 ft^2 exchanger with a heat transfer coefficient estimated[15.19] to be 250 BTU/hr/ft^2/°F.

To reduce costs, the distillation column and reflux accumulator were each constructed out of a carbon steel outer shell, with a 1/8 in thick inner 316 stainless steel lining. The reflux pump, condenser, and reboiler were constructed solely out of the 316 stainless steel. A shutdown pump, P-405, was also included to account for pumping the remaining liquid in the bottom of the column through to the next process section during a plant shutdown. With an assumed height equal to 6 ft

[15.18] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.
[15.19] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

of liquid remaining at the bottom of the column, the pump was designed to operate for 15 minute blocks once every shutdown, which was assumed to be once a day for 35 days out of the year. This pump is capable of producing a head of 63.3 ft, electrical utility of 0.8 kWh, and was also constructed of 316 stainless steel.

Section 15.1.5: Storage Tanks

Benzene Storage

Unit ID: TK-001	Temperature: 86 °F
Type: Storage Tank	Pressure: 0.2 psig
Material: 316 Stainless Steel	Height: 40 ft
Specification Sheet: Section 16, pg. 103	Diameter: 40 ft
Costing data: Section 17.1.5, pg. 111	

As discussed in Section 13.1, pg. 57 one day's worth of benzene is stored as excess raw material. Due to its low melting point of 41.9 °F, benzene is a liquid at ambient conditions. The volumetric flow of 1212.2 ft^3/hr was used with a volumetric safety factor of 1.67 to ensure that the tank never operates at full capacity for control and pressure considerations. The total storage volume was determined to be 48,584 ft^3. The tank is a conical roof storage vessel with a low pressure to be maintained with an N_2 control system. 316 stainless steel is used to ensure little corrosion due to the elements and possible pipeline impurities since benzene is highly toxic. Design calculations can be found in Appendix 4.6, pg. 221.

Phenol Storage

Unit ID: TK-501-2	Temperature: 113 °F
Type: Heated Storage Tank	Pressure: 0.2 psig
Material: 316 Stainless Steel	Height: 70 ft
Specification Sheet: Section 16, pg. 104	Diameter: 70 ft
Costing data: Section 17.1.5, pg.111	

As discussed in Section 13.6, pg. 62, two weeks' worth of phenol is stored as excess product in two storage tanks, each capable of maintaining up to a week's supply. The volumetric flow of 953.8 ft^3/hr was used with a volumetric safety factor of 1.67 to ensure that the tank never operates at full capacity for control and pressure considerations. The total storage volume was determined to be 267,588 ft^3 per tank. The tank is a conical roof storage vessel with a low pressure to be maintained with an N_2 control system. Due to the low melting point of phenol, the storage tank must be heated and insulated. Two-inch-thick insulation with a thermal conductivity of 0.4 BTU-in/hr/ft^2/°F was assumed to be the primary source of heat loss from each tank. Design calculations can be found in Appendix 4.6, pg. 221. With an insulation efficiency factor of 1.25, the total heat lost per tank was determined to be 155,166 BTU/hr. Allowing for a temperature drop to 105 °F, and heating up to 123 °F to achieve an average tank temperature of 113 °F , the tank is heated with a 4.25 ft^2 exchanger via thermal energy from 15 psig low pressure steam transferred to a pump-around flow of 20,226 lb/hr for each tank. The exchanger heat transfer coefficient was estimated[15.20] to be 250 BTU/hr/ft^2/°F. 316 stainless steel was used to combat corrosion from organic byproducts.

[15.20] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Byproduct Storage

Unit ID: TK-503	Temperature: 113 °F
Type: Heated Storage Tank	Pressure: 0.2 psig
Material: 316 Stainless Steel	Height: 15 ft
Specification Sheet: Section 16, pg. 105	Diameter: 15 ft
Costing data: Section 17.1.5, pg. 111	

As discussed in Section 13.6, pg. 62, one day's worth of byproducts is stored as partial furnace fuel. The volumetric flow of 71 ft^3/hr was used with a volumetric safety factor of 1.67 to ensure that the tank never operates at full capacity for control and pressure considerations. The total storage volume was determined to be 2841 ft^3. The tank is a conical roof storage vessel with a low pressure to be maintained with an N_2 control system. Due to the low melting point of phenol and the other byproducts, the storage tank must be heated and insulated. Two-inch-thick insulation with a thermal conductivity of 0.4 BTU-in/hr/ft^2/°F was assumed to be the primary source of heat loss from each tank. Design calculations can be found in Appendix 4.6, pg. 221. With an insulation efficiency factor of 1.25, the total heat lost was determined to be 7496 BTU/hr. Allowing for a temperature drop to 105 °F , and heating up to 123 °F to achieve an average tank temperature of 113 °F , the tank is heated with a 0.21 ft^2 exchanger via thermal energy from 15 psig low pressure steam transferred to a pump-around flow of 965 lb/hr. The exchanger heat transfer coefficient was estimated[15.21] to be 250 BTU/hr/ft^2/°F. 316 stainless steel was used to combat corrosion from organic byproducts.

[15.21] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Section 15.2: Minor Process Units

Section 15.2.1: Furnace

As discussed in section 14.1, pg. 65, the furnace H-001 is used to heat the heating oil from its temperature after cooling the reactor vessels up to the temperature necessary for reactor feed heating in E-202. A total of 32,776,592 BTU/hr is necessary to heat the oil in the furnace from 654 °F to 705 °F. 4,636,836 BTU/hr of that heat duty is achieved by burning the byproducts stored from stream 35. The remainder comes from burning natural gas fuel. Costing data can be found in Section 17.1.6, pg. 112.

Section 15.2.2: Flare System

Based on information from the U.S. Environmental Protection Agency (EPA) [15.22], the flare system represented in V-401 was designed with a 10 in tip diameter, 230 ft stack height, and derrick support structure. A kick back drum of 10 in diameter and L/D ratio of 2 was also used. 316 stainless steel piping and construction were used due to the high temperatures and possible corrosive elements present. Costing data can be found in Section 17.1.7, pg. 112.

Section 15.2.3: Process Heater

As discussed in Section 14.1, pg. 65, E-202 finishes heating the reactor feed up to 698 °F just above reaction conditions. The 77,555,400 BTU/hr transfer occurs in a 11,261 ft^2 exchanger

[15.22] Evans, L.B., W.M. Vatavuk, "VOC Destruction Controls", North Carolina, 2000.

with a heat transfer coefficient estimated[15.23] to be 30 BTU/hr/ft^2/°F. Design calculations can be found in Appendix 4.2.1, pg. 213. Costing data can be found in Section 17.1.3, pg. 109.

Section 15.2.4: Process Coolers

Steam Formation

Design calculations for the formation of steam in units E-301, E-303, E-501, and E-503 can be found in Appendix 4.2.1, pg. 213. The required areas for exchange are 600, 578, 536, and 6.7 ft^2 respectively with heat transfer coefficients estimated[15.24] to be 250 BTU/hr/ft^2/°F. For the purposes of costing, all exchangers below a minimum surface area were taken to be 150 ft^2 due to a lack of small exchanger estimating techniques. Low pressure 15 psig steam was produced for use in the heat integration network at a temperature of 285 °F. A temperature approach of 35 °F to the 285 °F saturation temperature was used to ensure the formation of nucleate boiling of the boiler feed water used for the conversion to steam. See Section 14.1, pg. 67 for a discussion of the amount of steam produced and its relevance to the heat integration network. 316 stainless steel tubes were used due to the high temperatures and possible corrosive elements present, while a carbon steel outer shell is acceptable for handling the boiler feed water evaporation to steam. Costing data can be found in Section 17.1.3, pg. 109.

[15.23] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.
[15.24] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Stream Coolers

Design calculations for the cooling process streams in units E-302, E-304, E-502, and E-504 can be found in Appendix 4.2.1, pg. 213. The required areas for exchange are 5325, 5370, 1037, and 81 ft^2 respectively with heat transfer coefficients estimated[15.25] to be 60 BTU/hr/ft^2/°F. For the purposes of costing, all exchangers below a minimum surface area were taken to be 150 ft^2 due to a lack of small exchanger estimating techniques. Cooling water is allowed to vary from 86 °F up to 104 °F as a conservative temperature change to minimize thermal pollution of wastewater. See Section 14.1, pg. 67 for a discussion of the amount of cooling water necessary. 316 stainless steel tubes were used due to the high temperatures and possible corrosive elements present, while a carbon steel outer shell is acceptable for handling the cooling water. Costing data can be found in Section 17.1.3, pg. 109.

[15.25] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

Section 16

Specification Sheets

Air Compressor

Identification: Item *Air Compressor* Date: *18 April 2017*
Item No. C-101-3 By: *BGR*
No. required 1

Function: Pressurize fresh air feed.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	86	384.1
Pressure (psig)	0.0	580.2
Vapor Fraction	1.0	1.0
Mass Flow (lb/hr)	56573	56573
Component Mass Flow (lb/hr)		
Benzene	-	-
Phenol	-	-
Catechol	-	-
Benzoic Acid	-	-
Benzaldehyde	-	-
Water	-	-
Oxygen	13120	13120
Nitrogen	43453	43453
Molar Flow (lbmol/hr)	1961	1961
Operating Volume Flow (cuft/hr)	780844	30162

Design Data:

Net Work: 4629 hp
Material of Construction: Cast Iron
No. Stages: 3
No. Intercoolers: 2
Net Heat Duty: -7,742,918 BTU/hr
Type: Multistage Compressor
Isentropic Efficiency: 0.85 per stage
Overall Compression ratio: 4

Utilities: Cooling Water at 430,162 lb/hr and Electricity at 3452 kWh

Comments and drawings: Intercoolers used to ensure structural stability of the multistage compressor
See Section 12 Process Flow Sheet Section 100

Feed Pump

Identification: Item *Feed Pump* Date: *18 April 2017*
Item No. P-101 By: *BGR*
No. required 1

Function: Pressurize fresh Benzene feed.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	86	92.1
Pressure (psig)	0.0	638.2
Vapor Fraction	0.0	0.0
Mass Flow (lb/hr)	65616	65616
Component Mass Flow (lb/hr)		
Benzene	65616	65616
Phenol	-	-
Catechol	-	-
Benzoic Acid	-	-
Benzaldehyde	-	-
Water	-	-
Oxygen	-	-
Nitrogen	-	-
Molar Flow (lbmol/hr)	840	840
Operating Volume Flow (cuft/hr)	1212	1217

Design Data:

Net Work: 95.85 hp
Material of Construction: Cast Iron
No. Stages: 2
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: HSC
Flowrate: 151.2 gpm
Head: 1698 ft
Max Motor hp: 1450

Utilities: Electricity at 71.4 kWh

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

Recycle Pump

Identification: Item *Recycle Pump* Date: *18 April 2017*
Item No. P-102 By: *BGR*
No. required 1

Function: Pressurize the Benzene recycle.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	172.4	176.6
Pressure (psig)	5.3	638.2
Vapor Fraction	0.0	0.0
Mass Flow (lb/hr)	453124	453124
Component Mass Flow (lb/hr)		
Benzene	452800	452800
Phenol	1	1
Catechol	-	-
Benzoic Acid	-	-
Benzaldehyde	-	-
Water	281	281
Oxygen	7	7
Nitrogen	35	35
Molar Flow (lbmol/hr)	4974	4974
Operating Volume Flow (cuft/hr)	7597	7621

Design Data:

Net Work: 457 hp
Material of Construction: 316 Stainless Steel
No. Stages: 2
Shaft rpm: 3600
Type: Centrifugal Pump
Orientation: HSC
Flowrate: 948 gpm
Head: 1787 ft
Max Motor hp: 1450

Utilities: Electricity at 340.2 kWh

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

Vapor Effluent Turbine

Identification: Item *Vapor Effluent Turbine* Date: *18 April 2017*
Item No. C-301 By: *BGR*
No. required 1

Function: Produce electricity from the large pressure drop.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	441.5	327.5
Pressure (psig)	575.6	155.0
Vapor Fraction	1.0	0.97
Mass Flow (lb/hr)	190451	190451
Component Mass Flow (lb/hr)		
Benzene	139430	139430
Phenol	8743	8743
Catechol	147	147
Benzoic Acid	6	6
Benzaldehyde	16	16
Water	158	158
Oxygen	1073	1073
Nitrogen	40878	40878
Molar Flow (lbmol/hr)	3381	3381
Operating Volume Flow (cuft/hr)	47368	152630

Design Data:

Net Work Recovered: 2858 hp
Material of Construction: 316 Stainless Steel
Pressure: 155 psig
Type: Gas Expander – Compression Design
Isentropic Efficiency: 0.85
Mechanical Efficiency: 0.98

Utilities: Produce Electricity at 2131 kWh

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

Liquid Effluent Turbine

Identification: Item *Liquid Effluent Turbine* Date: *18 April 2017*
Item No. P-301 By: *BGR*
No. required 1

Function: Produce electricity from the large pressure drop.

Operation: Continuous

Materials handled:	Feed	Discharge
Temperature (°F)	441.5	437.0
Pressure (psig)	575.6	155.0
Vapor Fraction	0.0	0.0
Mass Flow (lb/hr)	319246	319246
Component Mass Flow (lb/hr)		
Benzene	256770	256770
Phenol	57268	57268
Catechol	2087	2087
Benzoic Acid	146	146
Benzaldehyde	116	116
Water	146	146
Oxygen	103	103
Nitrogen	2610	2610
Molar Flow (lbmol/hr)	4021	4021
Operating Volume Flow (cuft/hr)	7892	7838

Design Data:

Net Work Recovered: 145 hp
Material of Construction: 316 Stainless Steel
Pressure: 155 psig
Type: Liquid Expander – Centrifugal Pump Design
Isentropic Efficiency: 0.6

Utilities: Produce Electricity at 108.1 kWh

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

Effluent Heat Exchanger

Identification: Item *Effluent Heat Exchanger* Date: *18 April 2017*
Item No. E-201 By: *BGR*
No. required 1

Function: Cool down reactor effluent while simultaneously pre-heating reactor feed.

Operation: Continuous

Materials handled:	Cold In	Cold Out	Hot In	Hot Out Vapor	Hot Out Liquid
Temperature (°F)	165	515.4	662	441.5	441.5
Pressure (psig)	638.2	636.4	580.1	575.6	575.6
Vapor Fraction	0.0	0.0	1.0	1.0	0.0
Mass Flow (lb/hr)	453124	453124	509697	190451	319246
Component Mass Flow (lb/hr)					
Benzene	452800	452800	396200	139430	256770
Phenol	1	1	66011	8743	57268
Catechol	-	-	2234	147	2087
Benzoic Acid	-	-	152	6	146
Benzaldehyde	-	-	132	16	116
Water	281	281	304	158	146
Oxygen	7	7	1176	1073	103
Nitrogen	35	35	43488	40878	2610
Molar Flow (lbmol/hr)	5814	5814	7402	3381	4021
Operating Volume Flow (cuft/hr)	8835	14402	127830	47368	7892

Design Data:

Effective Surface Area/unit: 8401.5 ft^2
LMTD: 122.76 °F
Heat Exchanged: 88,350,260 BTU/hr
Service Transfer Coeff: 85.67 BTU/(h-ft^2-°F)
Tube Side: Material of Construction: 316 Stainless Steel
No.: 700
OD: 0.75 in
Length: 360 in
Pitch: 0.9375 in
No. Passes/Shell: 2
Shell Side: Material of Construction: 316 Stainless Steel
ID: 40 in
OD: 42.21 in
No. Passes/Shell: 1

Type: DEU Horizontal
Shells in Parallel: 1
Shells in Series: 1
Shells/unit: 1

Comments and drawings: Hot Fluid on Tube Side
Has two nozzles for two phase hot stream out
See Section 12 Process Flow Sheet Section 200 and Appendix 4.2.2 TEMA Sheet

Reactor Vessels

Identification: Item *Reactor Vessels* Date: *18 April 2017*
Item No. R-201-4A/B By: *BGR*
No. required 5

Function: Allow the primary and secondary reactions to take place.

Operation: Continuous

Materials handled:	Feed	Overall Effluent
Temperature (°F)	665	662
Pressure (psig)	580.1	580.1
Vapor Fraction	1.0	1.0
Mass Flow (lb/hr)	509697	509697
Component Mass Flow (lb/hr)		
Benzene	452800	396200
Phenol	1	66011
Catechol	-	2234
Benzoic Acid	-	152
Benzaldehyde	-	132
Water	281	304
Oxygen	13127	1176
Nitrogen	43488	43488
Molar Flow (lbmol/hr)	7775	7402
Operating Volume Flow (cuft/hr)	138890	127830

Design Data:

Adiabatic Temperature Rise/unit: 54 °F
Mass catalyst/unit: 21,677 lb
Material of Construction: Carbon Steel outer shell with 316 Stainless Steel inner shell
Recommended inner diameter: 9.12 ft
Functional Height/unit: 9.12 ft
Total Functional Height: 36.5 ft
Total Reactor Volume: 2384 ft^3
Reactor Volume/unit: 596 ft^3
Total Reactor Pressure Drop: 8.55 psi
Reactor Pressure Drop/unit: 2.14 psi

No. units in series: 4
Orientation: Vertical
Bed Porosity: 0.42
Total Residence Time: 1.03 min
Residence Time/unit: 15.4 sec

Utilities: 14,926,269 BTU/hr removed per unit with 1,000,000 lb/hr heating oil

Comments and drawings: Assume reaction conversion is evenly spread out over all units
Intercoolers allow the temperature to oscillate +/-28 °F about the optimal isothermal operating temperature of 662 °F
Purchasing five units will allow for easy changing with less downtime
Feed pressure is sufficient such that average pressure across reactor is the optimal isobaric operating pressure of 580.2 psig
See Section 12 Process Flow Sheet Section 200

Flash Drum

Identification: Item *Flash Drum* Date: *18 April 2017*
Item No. T-301 By: *BGR*
No. required 1

Function: Separate non-condensables from desireable organics.

Operation: Continuous

Materials handled:	Feed 1	Feed 2	Vapor Exit	Liquid Exit
Temperature (°F)	110	110	110.1	110.1
Pressure (psig)	145.0	145.0	145.0	145.0
Vapor Fraction	0.45	0.02	1.0	0.0
Mass Flow (lb/hr)	190451	319246	47015	462673
Component Mass Flow (lb/hr)				
Benzene	139430	256770	3233	392960
Phenol	8743	57268	9	66002
Catechol	147	2087	-	2234
Benzoic Acid	6	146	-	152
Benzaldehyde	16	116	-	132
Water	158	146	8	296
Oxygen	1073	103	1108.3	68
Nitrogen	40878	2610	42656	830.8
Molar Flow (lbmol/hr)	3381	4021	1599	5803
Operating Volume Flow (cuft/hr)	60759	8668	60919	8422

Design Data:

Hold-up time: 5 min
Pressure: 145 psig
Functional height: 25.2 ft
Material of Construction: Carbon Steel outer shell with
316 Stainless Steel inner shell
Recommended inside diameter: 8.4 ft
Orientation: Horizontal
Frac. of Drum Full: 0.5
K-factor: 0.27
Vap Velocity Allowed: 8.38 ft/s
Liq. Vol Held: 701.6 ft^3

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

Distillation Column 1

Identification: Item *Distillation Column 1* Date: *18 April 2017*
Item No. T-302 By: *BGR*
No. required 1

Function: Separate Benzene and non-condensables from Phenol and other organics.

Operation: Continuous

Materials handled:	Feed	Liquid Dist.	Bottoms	Vapor Dist.
Temperature (°F)	110.1	172.4	389.8	172.4
Pressure (psig)	145.0	5.3	8.7	5.3
Vapor Fraction	0.0	0.0	0.0	1.0
Mass Flow (lb/hr)	462673	387469	68803	6369
Component Mass Flow (lb/hr)				
Benzene	392960	387180	284	5498
Phenol	66002	1	66001	-
Catechol	2234	-	2234	-
Benzoic Acid	152	-	152	-
Benzaldehyde	132	-	132	-
Water	296	281	-	14
Oxygen	68	7	-	61
Nitrogen	831	35	-	796
Molar Flow (lbmol/hr)	5803	4974	728	102
Operating Volume Flow (cuft/hr)	8422	7597	1201	33696

Design Data:

Number of trays: 32
Enriching Section: 14
Stripping Section: 18
Pressure: 8.8 psig
Functional height: 48 ft
Material of Construction: Carbon Steel outer shell with 316 Stainless Steel inner shell
Recommended inside diameter:
Enriching Section: 15.5 ft
Stripping Section: 17.5 ft
Average Tray efficiency: 0.32
Feed stage: 14

Molar reflux ratio: 0.50
Tray spacing: 1.5 ft
Skirt height: 17 ft

Utilities: Cooling water at 5,743,677 lb/hr and 500 psig steam at 163,029 lb/hr

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

Distillation Column 2

Identification: Item *Distillation Column 2* Date: *18 April 2017*
Item No. T-401 By: *BGR*
No. required 1

Function: Separate Phenol from Catechol and other organics.

Operation: Continuous

Materials handled:	Feed	Liquid Dist.	Bottoms	Vapor Dist.
Temperature (°F)	389.8	377.1	476.1	377.1
Pressure (psig)	8.7	5.3	8.8	5.3
Vapor Fraction	0.0	0.0	0.0	1.0
Mass Flow (lb/hr)	68803	65463	2684	656
Component Mass Flow (lb/hr)				
Benzene	284	256	-	28
Phenol	66001	65076	299	626
Catechol	2234	1	2233	-
Benzoic Acid	152	-	152	-
Benzaldehyde	132	130	-	2
Water	-	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Molar Flow (lbmol/hr)	728	696	25	7
Operating Volume Flow (cuft/hr)	1201	1139	44	3063

Design Data:

Number of trays: 20
Pressure: 8.8 psig
Functional height: 30 ft
Material of Construction: Carbon Steel outer shell with 316 Stainless Steel inner shell
Recommended inside diameter: 12 ft
Average Tray efficiency: 0.53
Feed stage: 8

Molar reflux ratio: 4.0
Tray spacing: 1.5 ft
Skirt height: 17 ft

Utilities: Cooling water at 3,877,717 lb/hr and 500 psig steam at 92,590 lb/hr

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

Distillation Column 3

Identification: Item *Distillation Column 3* Date: *18 April 2017*
Item No. T-402 By: *BGR*
No. required 1

Function: Separate Phenol from Benzaldehyde and other organics.

Operation: Continuous

Materials handled:	Feed	Liquid Dist.	Bottoms	Desired Side Product
Temperature (°F)	377.2	303.6	395.6	394.6
Pressure (psig)	15.3	5.3	10.0	9.7
Vapor Fraction	0.0	0.0	0.0	1.0
Mass Flow (lb/hr)	65463	2162	44	63255
Component Mass Flow (lb/hr)				
Benzene	256	255	-	1
Phenol	65076	1883	44.2	63148
Catechol	1	-	-	1
Benzoic Acid	-	-	-	-
Benzaldehyde	130	23.9	0.1	106
Water	-	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Molar Flow (lbmol/hr)	696	24	1	672
Operating Volume Flow (cuft/hr)	1140	37	1	243690

Design Data:

Number of trays: 22
Enriching Section: 16
Stripping Section: 6
Pressure: 8.8 psig
Functional height: 50 ft
Material of Construction: Carbon Steel outer shell with 316 Stainless Steel inner shell
Recommended inside diameter:
Enriching Section: 5.5 ft
Stripping Section: 7.5 ft
Average Tray efficiency: 0.82
Feed stage: 16
Side Product Stage: 20

Molar reflux ratio: 29.25
Tray spacing: 1.5 ft
Skirt height: 17 ft

Utilities: Cooling water at 860,802 lb/hr and 500 psig steam at 38,568 lb/hr

Comments and drawings: Most difficult separation due to close boiling components within 7 °F at operating pressure
See Section 12 Process Flow Sheet Section 400

Benzene Storage

Identification: Item *Benzene Storage* Date: *18 April 2017*
Item No. TK-001 By: *BGR*
No. required 1

Function: Store excess raw Benzene for production.

Operation: Continuous

Materials handled:	To Process
Temperature (°F)	86
Pressure (psig)	0.0
Vapor Fraction	0.0
Mass Flow (lb/hr)	65616
Component Mass Flow (lb/hr)	
Benzene	65616
Phenol	-
Catechol	-
Benzoic Acid	-
Benzaldehyde	-
Water	-
Oxygen	-
Nitrogen	-
Molar Flow (lbmol/hr)	840
Operating Volume Flow (cuft/hr)	1212

Design Data:

Amount of Benzene Stored: 1 day
Recommended inside diameter: 40 ft
Functional height: 40 ft
Material of construction: 316 Stainless Steel
Roof design: conical
Pressure: 6 in H_2O maintained with N_2 control system
Total storage volume: 48,584 ft^3

Comments and drawings: See Section 12 Process Flow Sheet Section 000

Phenol Storage

Identification: Item *Phenol Storage* Date: *18 April 2017*
Item No. TK-501-2 By: *BGR*
No. required 2

Function: Store excess product Phenol from production.

Operation: Continuous

Materials handled: From Process

Temperature (°F)	113
Pressure (psig)	0.0
Vapor Fraction	0.0
Mass Flow (lb/hr)	63256
Component Mass Flow (lb/hr)	
Benzene	1
Phenol	63148
Catechol	1
Benzoic Acid	-
Benzaldehyde	106
Water	-
Oxygen	-
Nitrogen	-
Molar Flow (lbmol/hr)	672
Operating Volume Flow (cuft/hr)	954

Design Data:

Amount of Phenol Stored: 7 days
Recommended inside diameter: 70 ft
Functional height: 70 ft
Material of construction: 316 Stainless Steel
Roof design: conical
Pressure: 6 in H_2O maintained with N_2 control system
Total storage volume: 267,588 ft^3
Insulation: 2 in thickness with thermal conductivity of 0.4 BTU-in/(h-ft^2-°F)
Heat Loss: 155,166 BTU/hr
Pumparound flow: 20,226 lb/hr

Utilities: 15 psig steam at 165 lb/hr

Comments and drawings: Heated storage used to prevent Phenol crystallization
See Section 12 Process Flow Sheet Section 500 and Appendix 4.6

Byproduct Storage

Identification: Item *Byproduct Storage* Date: *18 April 2017*
Item No. TK-503 By: *BGR*
No. required 1

Function: Store excess product Byproducts from production for use as furnace fuel.

Operation: Continuous

Materials handled: From Process

Temperature (°F)	113
Pressure (psig)	0.0
Vapor Fraction	0.0
Mass Flow (lb/hr)	4890
Component Mass Flow (lb/hr)	
Benzene	255
Phenol	2226
Catechol	2233
Benzoic Acid	152
Benzaldehyde	24
Water	-
Oxygen	-
Nitrogen	-
Molar Flow (lbmol/hr)	49
Operating Volume Flow (cuft/hr)	71

Design Data:

Amount of Phenol Stored: 1 day
Recommended inside diameter: 15 ft
Functional height: 15 ft
Material of construction: 316 Stainless Steel
Roof design: conical
Pressure: 6 in H_2O maintained with N_2 control system
Total storage volume: 2841 ft^3
Insulation: 2 in thickness with thermal conductivity of 0.4 BTU-in/(h-ft^2-°F)
Heat Loss: 7496 BTU/hr
Pumparound flow: 965 lb/hr

Utilities: 15 psig steam at 8 lb/hr

Comments and drawings: Heated storage used to prevent Byproduct crystallization
See Section 12 Process Flow Sheet Section 500 and Appendix 4.6

Section 17

Equipment Costing Summary

Table 17.1. Summary table for all process units including purchase cost, bare module factor, and bare module cost.

Process Equipment ID	Type	Purchase Cost ($)	Bare Module Factor	Bare Module Cost ($)
TK-001	**Storage**	$384,000	3.21	$1,360,000
P-101	**Process Machinery**	$53,300	3.30	$176,000
P-102	**Process Machinery**	$282,000	3.30	$931,000
P-301	**Process Machinery**	$98,900	3.30	$326,000
P-302	**Process Machinery**	$10,430	3.30	$34,400
P-303	**Other Equipment**	$11,500	3.30	$37,900
P-401	**Process Machinery**	$10,800	3.30	$35,600
P-402	**Other Equipment**	$9,320	3.30	$30,800
P-403	**Process Machinery**	$8,210	3.30	$27,100
P-404	**Process Machinery**	$8,280	3.30	$27,300
P-405	**Other Equipment**	$8,350	3.30	$27,600
C-101-3	**Fabricated Equipment**	$1,840,000	2.15	$3,960,000
C-301	**Fabricated Equipment**	$903,000	2.15	$1,940,000
T-301	**Fabricated Equipment**	$133,000	4.16	$553,000
T-302	**Fabricated Equipment**	$667,000	4.16	$2,780,000
T-401	**Fabricated Equipment**	$325,000	4.16	$1,350,000
T-402	**Fabricated Equipment**	$296,000	4.16	$1,230,000
R-201A	**Fabricated Equipment**	$209,000	4.16	$869,000
R-202A	**Fabricated Equipment**	$209,000	4.16	$869,000
R-203A	**Fabricated Equipment**	$209,000	4.16	$869,000
R-204A	**Fabricated Equipment**	$209,000	4.16	$869,000
R-20XB	**Spare**	$209,000	4.16	$869,000
E-101	**Fabricated Equipment**	$14,100	3.17	$44,700
E-102	**Fabricated Equipment**	$14,800	3.17	$44,700
E-201	**Fabricated Equipment**	$331,000	3.17	$1,050,000
E-202	**Fabricated Equipment**	$403,000	3.17	$1,280,000
E-203	**Fabricated Equipment**	$179,000	3.17	$567,000
E-204	**Fabricated Equipment**	$107,000	3.17	$339,000
E-205	**Fabricated Equipment**	$310,000	3.17	$983,000
E-301	**Fabricated Equipment**	$40,900	3.17	$129,000
E-302	**Fabricated Equipment**	$156,000	3.17	$495,000
E-303	**Fabricated Equipment**	$40,300	*3.17*	$128,000
E-304	**Fabricated Equipment**	$157,000	3.17	$498,000
E-305	**Fabricated Equipment**	$510,000	3.17	$1,620,000
E-306	**Fabricated Equipment**	$132,000	3.17	$418,000
E-401	**Fabricated Equipment**	$122,000	3.17	$387,000
E-402	**Fabricated Equipment**	$229,000	3.17	$726,000
E-403	**Fabricated Equipment**	$51,200	3.17	$162,000
E-404	**Fabricated Equipment**	$63,100	3.17	$200,000
E-501	**Fabricated Equipment**	$38,000	3.17	$121,000
E-502	**Fabricated Equipment**	$50,700	3.17	$161,000
E-503	**Fabricated Equipment**	$34,900	3.17	$111,000
E-504	**Fabricated Equipment**	$34,900	3.17	$111,000
E-505	**Fabricated Equipment**	$34,900	3.17	$111,000
E-506	**Fabricated Equipment**	$34,900	3.17	$111,000
E-507	**Fabricated Equipment**	$34,900	3.17	$111,000
V-301	**Fabricated Equipment**	$61,800	4.16	$257,000
V-401	**Fabricated Equipment**	$103,000	1.92	$197,000
V-402	**Fabricated Equipment**	$65,500	4.16	$273,000
V-403	**Fabricated Equipment**	$39,100	4.16	$163,000
TK-501	**Storage**	$905,000	3.21	$3,190,000
TK-502	**Storage**	$905,000	3.21	$3,190,000
TK-503	**Storage**	$87,900	3.21	$311,000
H-001	**Fabricated Equipment**	$992,000	2.19	$2,170,000
Total Costs	**-**	**$12,400,000**	**-**	**$38,800,000**

To begin plant operation, we request a total capital investment (TCI) of $83.6MM. $65.3MM of the total capital required will be spent on contractor fees, site preparation, service facilities, all process machinery, the land for the plant, royalties to the patent owners, as well as plant start-up costs, such as filling the purchased reactor vessels with the necessary amount of catalyst. More than half of this portion of the TCI will be allocated towards purchasing and installing all required pieces of equipment.

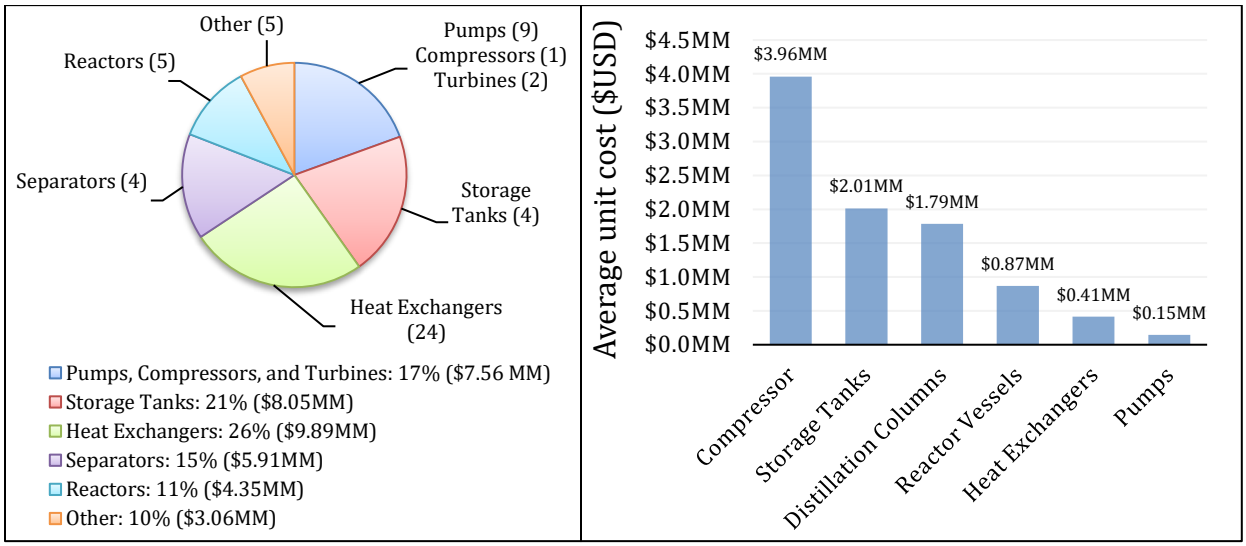


Figure 17.1. Breakdown of total equipment costs required for plant construction and the average equipment cost per vessel. Heat exchangers and pumps comprise a large portion of the fixed investment due to their abundance in the process, though they have the lowest average costs. The compressor, storage tanks, and distillation columns make up the most expensive units in the process due to size.

Of the $38.8MM required for all pieces of equipment, heat exchangers (26%), storage tanks (21%), and the pumps and compressors (17%) make up the bulk of the total equipment costs. The high equipment costs of the heat exchangers and pumps are a result of the sheer number of these vessels that appear in the process, though the most expensive pieces of equipment are the compressor, storage tanks, and distillation columns with average costs of $3.96MM, $2.01MM, and $1.79MM, respectively.

The most expensive piece of equipment is C-101-3, the $3.96MM three-stage air compressor required to bring ambient air to the ideal reactor operating pressure of 580 psig. This unit requires 4630hp. The first distillation column, T-302, responsible for separating most of the unreacted benzene from the desired phenol product, is the most expensive column due to size. It handles the largest volume of material following separation of the non-condensables in the flash drum and has a total height of 65 ft with an average diameter of 16.5 ft. Each of the two phenol storage tanks totals $3.19MM and the benzene storage tank will cost $1.36MM. The volume requirements for these tanks are responsible for their large bare module costs.

Section 17.1: Unit Costing Considerations

Section 17.1.1: Pumps, Compressors, and Turbines

The compressor, pumps, and turbines were costed in accordance with the equations presented in Chapter 16 of *Seider et. al, 2017*. Purchase cost calculations for each unit required the flow rates in gallons per minute of the respective stream through each unit, the head in feet for each pump, as well as the compressor horsepower. Each input was retrieved from the ASPEN process simulation results. The specific values used for equipment costing can be found in either the stream results for each pump, block results for the compressors, or unit descriptions in Section 15.1.1, pg. 71.

Section 17.1.2: Heat Exchangers, Reboilers, Condensers, and Reflux Accumulators

All heat exchangers were costed according to their required surface area and material of construction, discussed in Section 15.2, pg. 88. The effluent heat exchanger was costed in ASPEN.

These variables were used in accordance with the equations presented in *Seider et. al, 2017* to accurately determine the cost for each exchanger. The same methodology was applied for distillation column reboilers and condensers.

Reflux accumulators were treated as horizontal pressure vessels with holding times of five minutes. The vapor and liquid densities, as well as the volumetric flow rates into each accumulator, were taken from ASPEN profile data from the corresponding distillation column. The accumulators were assumed to have an aspect ratio of 2, and their costs were determined from the horizontal pressure vessel equation from Chapter 16 of *Seider et. al, 2017.* Detailed calculations can be found in Appendix 4.5, pg. 219.

Section 17.1.3: Reactor Vessels

The required volume for reactors R-201A, 202A, 203A, 204A, and 20XB was determined as described in Section 15.1.3, pg. 76. Each reactor vessel was treated as a vertical pressure vessel with a carbon steel base shell and a 1/8-inch stainless steel inner shell. The length and diameter of each partitioned reactor were used in combination with equations found in Chapter 16 of *Seider et. al, 2017* to determine an estimate of the bare module costs of the carbon steel outer vessels and stainless steel shells.

Section 17.1.4: Distillation Columns and Flash Drum

Our team consulted Professor Fabiano on the correct approach for sizing flash drum T-301. The calculations for determining drum size required the inlet flow rate to the vessel, the vapor and liquid fractions of the total inlet stream, the liquid and vapor densities of the inlet stream, avapor velocity design K factor of 0.27 (described in Section 15.1.4, pg. 78), an L/D ratio of 3, and a

holding time of five minutes. Calculation of the vessel dimensions from these parameters can be found in Appendix 4.4, pg. 218. This vessel was costed as a horizontal pressure vessel according to equations found in Chapter 16 of *Seider et. al, 2017.*

Each of the three distillation columns, T-302, 401, and 402, were first modeled in ASPEN to provide an initial estimate for the number of theoretical stages, as described in section 15.1.4, pg. 78. To develop an accurate estimate of tray column size, Murphree tray efficiencies were determined for each column using O'Connell correlations. The actual number of trays required for each column was calculated using the theoretical number of stages in combination with the calculated tray efficiencies. An example of this calculation can be found in Appendix 4.5, pg. 219. Using an assumed tray spacing of 1.5 ft, 3 ft spacing required for the feed tray, and an additional 4 ft and 10 ft for the enriching and stripping sections skirts, respectively, total column diameters and lengths for each tower were determined. These values were used in accordance with Chapter 16 of *Seider et. al, 2017* to accurately determine the cost of each column. Interior stainless steel shells were also costed, with a shell thickness of 1/8 inch, as discussed in Section 15.1.4, pg. 78, to prevent against the potentially corrosive properties of the reaction products.

Section 17.1.5: Storage Tanks

Storage tanks TK-001, 501, 502, and 503 were each costed using the storage tank pricing equation from Chapter 16 of *Seider et. al, 2017,* in accordance with the assumed volume of storage required for sufficient chemical inventory as described in Section 15.1.5, pg. 85. The insulation cost for each tank was assumed to be 10% of the tank's bare module cost. Design calculations for the pump-arounds for each tank, found in Appendix 4.6, pg. 221, determined that the required surface area for these exchangers was much less than the 150 ft^2 threshold for using costing

equations from Chapter 16 of *Seider et. al, 2017*. The costs for these exchangers were estimated by the minimum heat exchanger cost found in Chapter 16 of *Seider et. al, 2017*. For a detailed description of phenol tank insulation and pump-arounds, see Section 15.1.5, pg. 85.

Section 17.1.6: Hot Oil Furnace

The cost of the hot oil furnace, H-001, can be solely determined from the required heat duty of the unit. The heat duty of the furnace was calculated to be 32,776,592 BTU/hr and was used in accordance with *Seider's et. al, 2017* equations to determine purchase cost. See Section 15.2, pg. 88 for further details.

Section 17.1.7: Flare System

The flare system, V-401, was valued according to its physical dimensions discussed in Section 15.2.2, pg. 88. The flare purchase cost was determined according to methods suggested in *Evans et. al, 2000*, which relates flare purchase cost to diameter, length, and tip length via the Derrick-Guy Support Group equation taken from EPA recommendations[17.1].

[17.1] Evans, L.B., W.M. Vatavuk, "VOC Destruction Controls", North Carolina, 2000.

Section 18

Fixed-Capital Investment Summary

The methods used to estimate the total capital investment for the project from the total equipment purchase costs are shown in Table 18.1. The bare module factors for all fabricated equipment, process machinery, storage tanks, and spare plant parts are displayed in Table 17.1. The total purchase cost for all equipment was calculated to be $12.4MM and the total bare module cost is $38.8MM.

Table 18.1. Relationship between total capital investment, total permanent invest, and estimated equipment purchase costs (*Seider et. al, 2017).*

Total bare-module costs for fabricated equipment	C_{FE}					
Total bare-module costs for process machinery	C_{PM}					
Total bare-module costs for spares	C_{spare}					
Total bare-module costs for storage and surge tanks	$C_{storage}$					
Total cost for initial catalyst charges	$C_{catalyst}$					
Total bare-module costs for computers and software, including distributed control systems, instruments, and alarms	C_{comp}					
Total bare-module investment, TBM		C_{TBM}				
Cost of site preparation		C_{site}				
Cost of service facilities		C_{serv}				
Allocated costs for utility plants and related facilities		C_{alloc}				
Total of direct permanent investment, DPI			C_{DPI}			
Cost of contingencies and contractor's fee			C_{cont}			
Total depreciable capital, TDC				C_{TDC}		
Cost of land				C_{land}		
Cost of royalties				C_{royal}		
Cost of plant startup				$C_{startup}$		
Total permanent investment, TPI					C_{TPI}	
Working capital					C_{wc}	
Total capital investment, TCI						C_{TCI}

The factors used to determine the required costs for plant preparation, startup, product distribution, and royalties are shown in Table 18.2. These calculations formed the basis for calculating the total capital investment required for the project.

Table 18.2. Correlations between total capital investment and required fees for the proposed plant (*Seider et. al, 2017).*

Component of Total Capital Investment	**Relationship to C_{TCI}**
Cost of Site Preparation	20% of Total Bare Module Cost
Cost of Service Facilities	5% of Total Bare Module Cost
Cost of Contingencies and Contractor's Fee	18% of Direct Permanent Investment
Cost of Land	2% of Total Depreciable Capital
Cost of Initial Royalty for Patent Data	2% of Total Depreciable Capital
Cost of Plant Startup	10% of Total Depreciable Capital

A breakdown of the required investment costs, beginning with total bare module costs and ending with the required total capital investment for the project, is shown in Table 18.3. Our team requests an initial investment of $65.3MM to cover the minimum required costs to build the phenol production plant.

Table 18.3. Calculation of total capital investment required from estimated equipment bare module costs (*Downey, 2008).*

Investment Summary				
Total Bare Module Costs:				
Fabricated Equipment	$	28,257,400		
Process Machinery	$	1,557,400		
Spares	$	869,000		
Storage	$	8,051,000		
Other Equipment	$	96,300		
Catalysts	$	-		
Computers, Software, Etc.	$	-		
Total Bare Module Costs:			$	38,831,100
Direct Permanent Investment				
Cost of Site Preparations:	$	7,766,220		
Cost of Service Facilities:	$	1,941,555		
Allocated Costs for utility plants and related facilities:	$	-		
Direct Permanent Investment			$	48,538,875
Total Depreciable Capital				
Cost of Contingencies & Contractor Fees	$	8,736,998		
Total Depreciable Capital			$	57,275,873
Total Permanent Investment				
Cost of Land:	$	1,145,517		
Cost of Royalties:	$	1,145,517		
Cost of Plant Start-Up:	$	5,727,587		
Total Permanent Investment - Unadjusted			$	65,294,495
Site Factor				1.00
Total Permanent Investment			$	65,294,495

Section 19

Operating Costs – Cost of Manufacturing

Section 19.1: Variable Operating Costs

Table 19.1. Estimated raw material pricing and yearly requirements.

Raw Material	**Estimated Cost ($/lb)**	**Yearly Requirement (lb)**	**Total Annual Cost ($MM/yr)**
Benzene	($0.499)	520MM	($260MM)
Copper Chromium Oxide Catalyst	($65.8)	0.173MM	($12.0MM)
Catalyst Pelleting	($3.29)	-	($0.60MM)
Total	**-**	**-**	**($272MM)**

The fresh benzene feedstock for the process is available on site for a cost of $1,100/metric ton. After engaging in direct conversations with Yingkou Tanyun Chemical Research Institute in Shenzhen, China, we determined that the copper chromium oxide catalyst can be procured in bulk for $65.8/lb. We assumed a 5% markup on this cost for pelletization of the catalyst, which is necessary for use in a packed bed reactor.

Based on reactor design calculations, found in Appendix 4.3, pg. 216, it was found that each of the four reactor sections would require 21,700 lb catalyst, amounting to 86,800 lb to fill the entire reactor. In accordance with recommendations from industrial consultants, we assume the catalyst cannot be regenerated and has a 6-month lifespan. The reactor will require two fresh batches of catalyst each year, amounting to a yearly requirement of approximately 174,000 lb of catalyst.

Table 19.2. Utility cost estimates per hour and per operating year. Steam is produced in excess and sold for a profit.

Utilities	**Cost or Value ($)**	**Required Ratio (per lb phenol)**	**Cost ($/hr)**	**Total Cost ($/op-yr)**
High Pressure Steam (500psig)	($0.0085)/lb	4.65	($2,500)	($19.8MM)
Low Pressure Steam (15psig)	$0.0055/lb	0.92	$321	$2.50MM
Boiling Feed Water	($2.4 x 10^{-4})/lb	0.93	($14)	($112,000)
Cooling Water	($1.2 x 10^{-5})/lb	221	($167)	($1.30MM)
Electricity	$0.07/kWh	0.026	($14)	($0.90MM)
Natural Gas Fuel	($3.2 x 10^{-6})/BTU	603	($122)	($1.00MM)
Total	**-**	**-**	**($2,600)**	**($20.6MM)**

Referring to Table 14.2, our process generates 58,600 lb of low pressure steam/hr assuming all of the boiler feed water is successfully vaporized. Our process only requires 336 lb/hr of low pressure steam to maintain the phenol and byproduct storage tanks at an average temperature of 113 °F. The remaining 58,300 lb/hr of low pressure steam generated will be sold on site at a price of 6 cents per pound, generating a yearly revenue of $2.5MM.

Table 19.3. Annual general expense data required for plant operation (Chapter 17 of *Seider et. al 2017).*

Component of General Expenses	**Relationship to Sales**	**Total Annual Cost ($MM/yr)**
Selling and Transfer Expenses	2.0% of Sales	($13.6MM)
Direct Research	4.8% of Sales	($21.8MM)
Allocated Research	0.50% of Sales	($2.27MM)
Administrative Expenses	2.0% of Sales	($9.09MM)
Management Incentive Compensation	1.3% of Sales	($5.68MM)
Total	**10.6% of Sales**	**($52.5MM)**

General expense data required for plant operation in Table 19.3 is taken from *Seider et. al, 2017.* The combination of raw material costs, utilities, and general expenses for plant operation total to $344MM in annual variable costs.

Section 19.2: Fixed Operating Costs

Table 19.4. Fixed operating expenses required per year to carry out the duties at the plant site taken from Chapter 17 of *Seider et. al 2017*.

Operations (labor-related)	**Estimated Cost**	**Total Annual cost ($MM/yr)**
Direct Wages and Benefits	$40/operator hour	($0.832MM)
Direct Salaries and Benefits	15% Direct Wages and Benefits	($0.125MM)
Operating Supplies and Services	6% Direct Wages and Benefits	($0.499MM)
Technical Assistance to Manufacturing	$60,000/yr/operating shift	($0.600MM)
Control Laboratory	$65,000/yr/operating shift	($0.650MM)
Total	**-**	**($2.26MM)**

To ensure successful plant operation, we assumed we would need five daily operating shifts, each lasting approximately 4.8 hours. We also assumed employment of two operators per shift. These assumptions were aligned with suggestions from Table 17.3 in Chapter 17 *of Seider et. al. 2017* for a large continuous fluid generating process.

Table 19.5. Site maintenance cost estimates based on assumptions from Chapter 16 of *Seider et. al. 2017*.

Site Maintenance	**Estimated Cost**	**Total Annual Cost ($/yr)**
Wages and Benefits	4.5% Total Depreciable Capital	($2.58MM)
Salaries and Benefits	25% Maintenance Wages and Benefits	($0.644MM)
Materials and Services	100% Maintenance Wags and Benefits	($2.58MM)
Maintenance Overhead	5% Maintenance Wages and Benefits	($0.129MM)
Total	**-**	**($5.93MM)**

Table 19.6. Yearly general expense estimates based on assumptions from Chapter 16 *of Seider et. al. 2017.*

General Expenses	**Estimated Cost**	**Annual Cost**
General Plant Overhead	7.1% Maintenance Operations Wages and Benefits	($0.297MM)
Mechanical Department Services	2.4% Maintenance Operations Wages and Benefits	($0.100MM)
Employee Relations Dpt.	5.9% Maintenance Operations Wages and Benefits	($0.247MM)
Business Services	7.4% Maintenance Operations Wages and Benefits	($0.309MM)
Property Tax and Insurance	2% Total Depreciable Capital	($1.15MM)
Licensing Fees	3% of Total Annual Sales	($12.3MM)
Total	**-**	**($14.4MM)**

The combination of fixed operating expenses, site maintenance costs, and general yearly expenses, outlined in Tables 19.4-19.6, total $22.6MM in annual fixed operating costs.

Section 20

Profitability Analyses – Business Case

The novel oxidation reaction herein described for generating phenol in a 1:1 molar ratio from benzene with limited byproducts displays great potential as a profitable venture in the petrochemical industry. However, our team must obtain the necessary investments required to build the plant and begin production.

Of the $83.6MM capital investment, $18.3MM can be attributed to the present value of the project's working capital requirements, or the fixed capital and startup funds needed for the process to meet its goals until payments for phenol can be received. Working capital is composed of current assets, such as stored phenol inventory, and current liabilities, such as accounts payable for purchasing of the process feedstocks (*Seider et. al, 2017)*. The working capital ratio, highlighted in Table 20.1, is equal to $\frac{current\ assets\ (\$)}{current\ liabilities\ (\$)}$. Our project displays a ratio of 2.42 for the first three years of production, indicating the project's capacity to pay investors back in the short term.[20.1]

Table 20.1. Summary of working capital requirements and working capital ratio for the proposed project over the first three years of production.

Working Capital			
	2020	2021	2022
Accounts Receivable	$ 16,811,763	$ 8,405,881	$ 8,405,881
Cash Reserves	$ 1,141,612	$ 570,806	$ 570,806
Accounts Payable	$ (10,793,367)	$ (5,396,683)	$ (5,396,683)
Phenol Inventory	$ 7,845,489	$ 3,922,745	$ 3,922,745
Raw Materials	$ 334,403	$ 167,201	$ 167,201
Total	**$ 15,339,901**	**$ 7,669,950**	**$ 7,669,950**
Present Value at 15%	*$ 10,086,234*	*$ 4,385,319*	*$ 3,813,321*
Working Capital Ratio	**2.42**	**2.42**	**2.42**
Total Capital Investment			**$ 83,579,368**

[20.1] Picardo, Elvis. "Working Capital." *Investopedia*. N.p., 23 Aug. 2016. Web. 15 Apr. 2017.

The catalytic technology that drives this project will require the remainder of the current calendar year for additional research and process design, followed by three years of plant construction before any phenol product can be generated and distributed. Our team estimated the value of this project over a fifteen-year plant lifespan. The first two years of plant operation will be carried out at 50% of the 500MM lb/yr total phenol production capacity, and the remaining thirteen years at 90% production capacity.

Table 20.2 displays an overview of multiple profitability metrics for the process in its third production year, or the first year when the plant can operate at its maximum production capacity. Over the plant's first fifteen years of life, our team projects an internal rate of return (IRR) equal to 29.2%, nearly twice the nominal interest rate of 15%, as well as a return on investment (ROI) of 44.7%.

It is important to note that IRR assumes that all future cash inflows will be reinvested at the same rate of return. The IRR metric can be a confounding metric for new *product* developments, as single products are unlikely to generate increasing amounts of revenue over long periods of time.[20.2] Usually, peak sales are reached within a few years of launch, and demand dwindles as new products enter the market and competition increases. However, for our new, direct phenol generation *process*, it is highly likely that additional research and plant optimization will occur over time and improve plant capacity as well as product purity. Given the potential for process improvement, our team expects future cash flows to be reinvested with return rates even greater than the estimated IRR.

[20.2] Klleher, John C., and Justin J. MacCormack. "Internal Rate of Return: A Cautionary Tale." McKinsey & Company, Aug. 2004. Web. 16 Apr. 2017.

Table 20.2. Profitability metrics for the proposed process using base case pricing suggestions and a nominal interest rate of 15%.

Profitability Measures		
The Internal Rate of Return (IRR) for this project is		29.18%
The Net Present Value (NPV) of this project in 2017 is		$ 90,202,600
ROI Analysis (Third Production Year)		
Annual Sales	409,086,229	
Annual Costs	(332,443,645)	
Depreciation	(5,223,560)	
Income Tax	(28,567,610)	
Net Earnings	42,851,415	
Total Capital Investment	95,974,296	
ROI	44.65%	

To provide context for these metrics, DuPont's stock has increased 26.2% over the last three years for an annual growth rate of 8.7%, while the S&P index has grown 23.6% over the last three years for an annual growth rate of 7.9%.[20.3] This project presents the opportunity for a 44.7% ROI over three years, or 14.9% average annual return. This renders it as an attractive investment with greater potential than other investments in the chemical industry as well as other Fortune 500 companies.[20.4]

These compelling financials suggest that there is a profitable and realistic process design capable of producing phenol without comparable amounts of co-products. The value of this process is not reliant on the sale of low value byproducts produced from the intrinsic reaction chemistry, as it is in the conventional Hock process. The development of this disruptive catalytic technology will undoubtedly create ripples in the phenol marketplace. Any new technological

[20.3] "Summary for E.I. Du Pont De Nemours and Com - Yahoo Finance." *Yahoo!* Yahoo!, 2017. Web. 15 Apr. 2017.
[20.4] Summary for S&P 500 Yahoo Finance." *Yahoo!* Yahoo!, 2017. Web. 15 Apr. 2017.

undertaking is associated with risk, but the large payoff from this process warrants attention from investors.

The net present value (NPV) of the base case for the process over fifteen years was estimated to be $90MM. This project NPV assumes that all phenol produced is sold at $0.91/lb, generating constant yearly revenue streams of ~$409MM beginning in the third production year. A graph of the cumulative free cash flow for this process over time is shown in Figure 20.1.

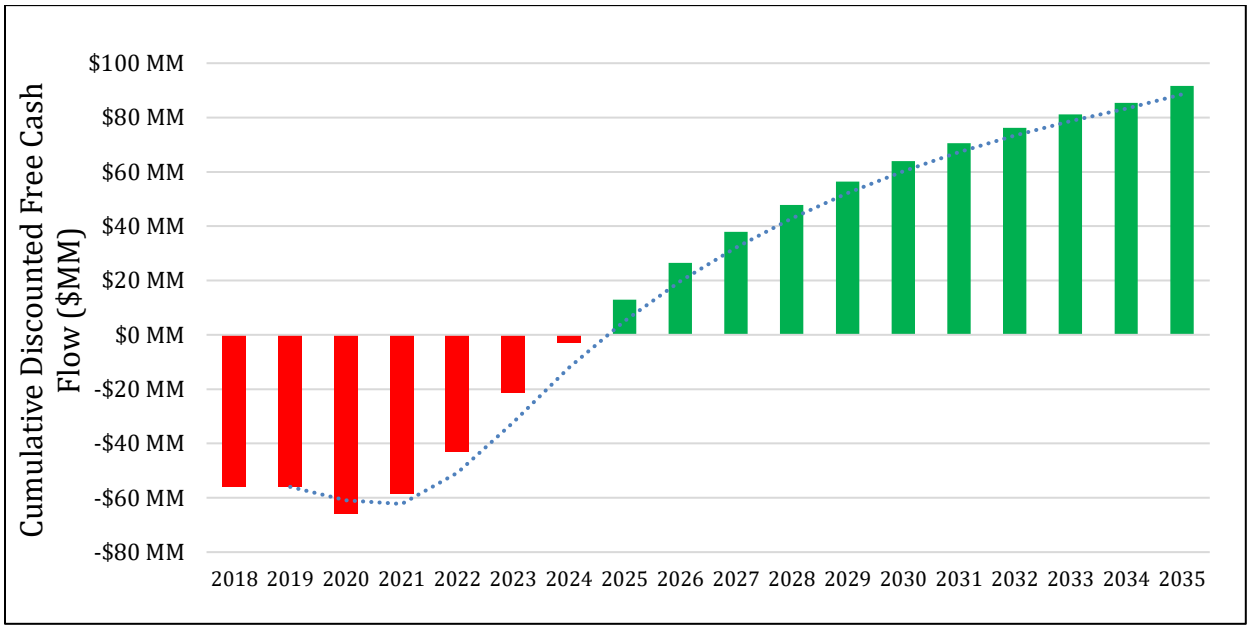


Figure 20.1. Cumulative discounted free cash flow ($MM) for project over fifteen-year lifespan assuming benzene price $0.50/lb and phenol price $0.91/lb. The process is shown to break-even in 2025, two years after reaching maximum production capacity.

The cumulative free cash flow graphic illustrates the value of the phenol production process in millions of 2017 dollars over time. In the first few years, the process nets a negative cash inflow due to site construction and plant development concomitant with an absence of phenol production and sales. Phenol sales will begin in 2021 with maximum production capacity achieved in 2023. The outlook for the process is promising. The process value breaks even in Q1 2025, two years after maximum capacity is reached, and displays sustained growth in the following decade.

Table 20.3. Summary of the depreciation schedule and annual earnings, costs, and taxes used to calculate yearly cash flows for the project.

Cash Flow Summary

Year	Percentage of Design Capacity	Sales	Capital Costs	Working Capital	Var Costs	Total Costs	Fixed Costs	Depreciation	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value at 15%
2017	0%	-	-	-	-	-	-	-	-	-	-	-	-
2018	0%	-	(65,294,500)	-	-	-	-	-	-	-	-	(65,294,500)	(56,777,800)
2019	0%	-	-	-	-	-	-	-	-	-	-	-	(56,777,800)
2020	0%	-	-	(15,339,900)	-	-	-	-	-	-	-	(15,339,900)	(66,864,100)
2021	45%	204,543,100	-	(7,670,000)	(154,944,000)	(177,499,618)	(22,555,600)	(11,455,200)	15,588,300	(6,235,300)	9,353,000	13,138,200	(59,352,200)
2022	68%	306,814,700	-	(7,670,000)	(232,416,000)	(254,971,631)	(22,555,600)	(18,328,300)	33,514,800	(13,405,900)	20,108,900	30,767,200	(44,055,500)
2023	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	(10,997,000)	65,645,600	(26,258,200)	39,387,400	50,384,300	(22,273,000)
2024	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	(6,598,200)	70,044,400	(28,017,800)	42,026,600	48,624,800	(3,993,100)
2025	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	(6,598,200)	70,044,400	(28,017,800)	42,026,600	48,624,800	11,902,400
2026	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	(3,299,100)	73,343,500	(29,337,400)	44,006,100	47,305,200	25,349,500
2027	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	36,716,500
2028	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	46,600,700
2029	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	55,195,800
2030	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	62,669,700
2031	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	69,168,800
2032	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	74,820,200
2033	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	79,734,400
2034	90%	409,086,200	-	-	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	45,985,600	84,007,600
2035	90%	409,086,200	-	30,679,800	(309,888,100)	(332,443,645)	(22,555,600)	-	76,642,600	(30,657,000)	45,985,600	76,665,400	90,202,600

Section 20.1: Sensitivity Analyses

Aside from the small-scale work performed by the team at CSIR, additional research has yet to be carried out to determine the accuracy of the patented data. Testing at a proper pilot plant must be performed to properly assess the viability of each assumption presented in this report. It is highly likely that industrial scale data collection from this process will elucidate problems with the current design that warrant increased funding. Although the previous economic analyses only presented the base case, Figure 20.2 presents a sensitivity for the impact of increased variable and capital costs on project value.

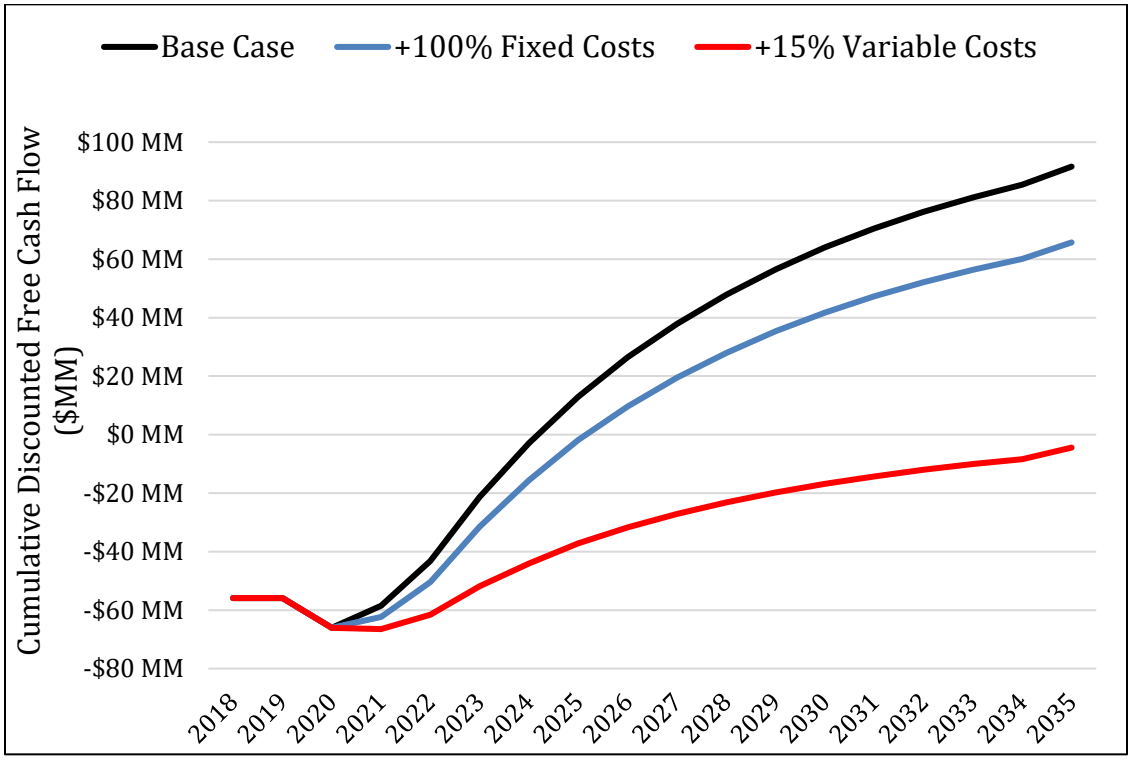


Figure 20.2. Cumulative discounted cash flows for the project with sensitivities for a 100% increase in fixed costs and 15% increase in variable costs compared to the base case. A 15% increase in variable costs results in a net loss of $5.43MM.

This graph displays the comparative impact of a 100% increase in fixed costs and 15% increase in variable costs on cumulative NPV. The impact on value for a 100% increase in fixed

costs is marginal, even when compared to a 15% increase in variable costs. These results indicate that project value will not be greatly affected if equipment costing data is inaccurate.

On the contrary, a slight increase in variable costs has a markedly greater impact on project value. The profitability of this process hinges much more on changes in variables costs, such as raw material prices, as opposed to equipment valuations, site construction costs, contractor fees, and the like.

Benzene feedstock composes the bulk of the annual variable costs associated with this process primarily due to the large design production capacity. Catalyst cost is less because of its long assumed lifetime.

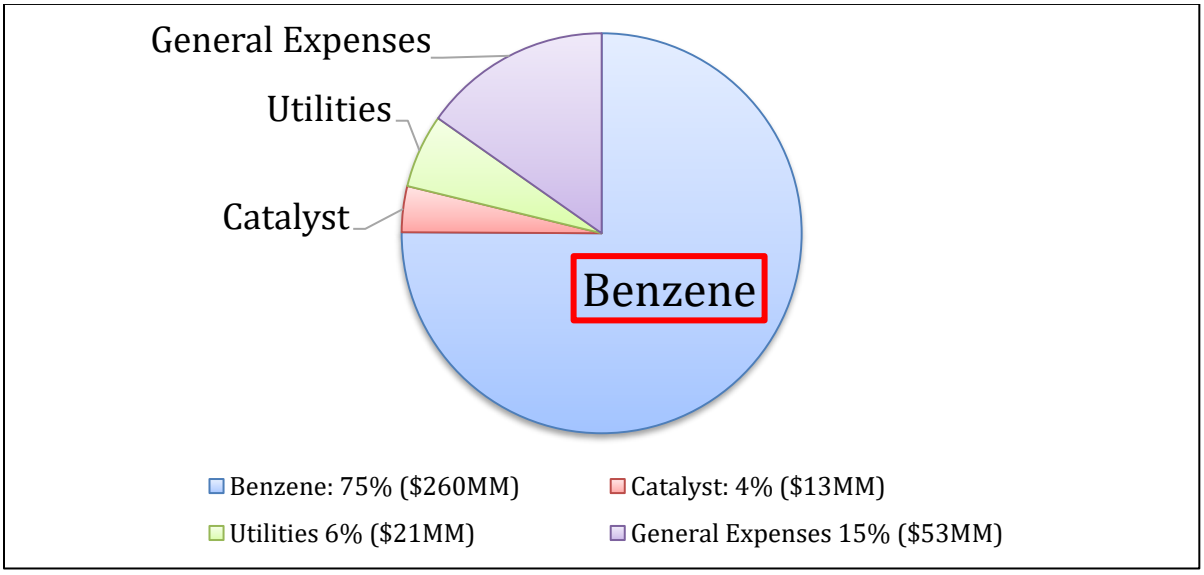


Figure 20.3. Annual variable cost distribution for direct benzene to phenol oxidation reaction assuming prices predicted by our marketing team. Benzene poses a serious threat to project value because it composes 75%, or $260MM, of all variable costs.

Because benzene constitutes 75% of the total variable costs for the process each year, the process' ability to recover any unreacted benzene greatly affects project value. Moreover, it was previously noted that total benzene conversion in the reactor is only 12.5%. The process recycle

stream must recover a substantial portion of the unreacted benzene to ensure the process is profitable. As it currently stands, our process recovers 97.7% of the total unreacted benzene. Our team generated a sensitivity analysis surrounding this crucial metric and used it as a primary guideline for process design.

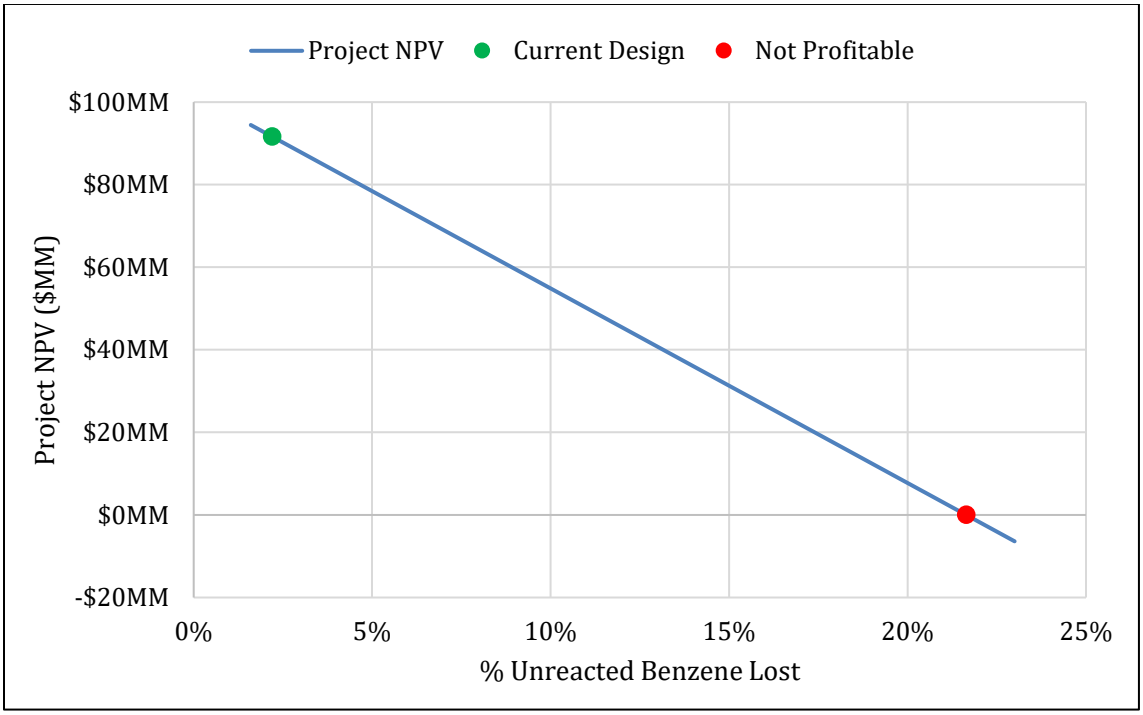


Figure 20.4. Effects of unreacted benzene lost in downstream separations on project NPV. Process profitability necessitates an overall unreacted benzene recovery above 79% (or less than 21% unreacted benzene lost).

Figure 20.4 predicts an extreme dependency on recovery of the unreacted benzene for process profitability. The red point indicates that if 21.3% of the unreacted benzene is not recovered in the recycle, the process is no longer profitable. Our downstream must recover at least 78.7% of the total unreacted benzene. The green point indicates the current percent of unreacted benzene lost with our process design: 2.2%. Because the amount of recovered benzene emerged as such an important factor for value creation, it dictated much of our process synthesis decision-

making. Any improvements or changes in the system that are required following a plant pilot run should seek to maximize unreacted benzene recovery in the recycle.

Each of the previous profitability analyses and sensitives accounted for variables intrinsic to the process. They assumed no variations in the benzene or phenol petrochemical market that might result in pricing changes and, correspondingly, a drastic change in project value. Assuming phenol and benzene prices aligned with suggestions from our marketing team, this process would still be profitable selling phenol at $0.79/lb. Holding benzene price constant, this is equivalent to a 13.2% decrease in the suggested price for phenol. If phenol prices remain as provided, the project would remain profitable until the price of benzene exceeds $0.59/lb. This corresponds to a 19.1% increase in the price of benzene suggested for this project.

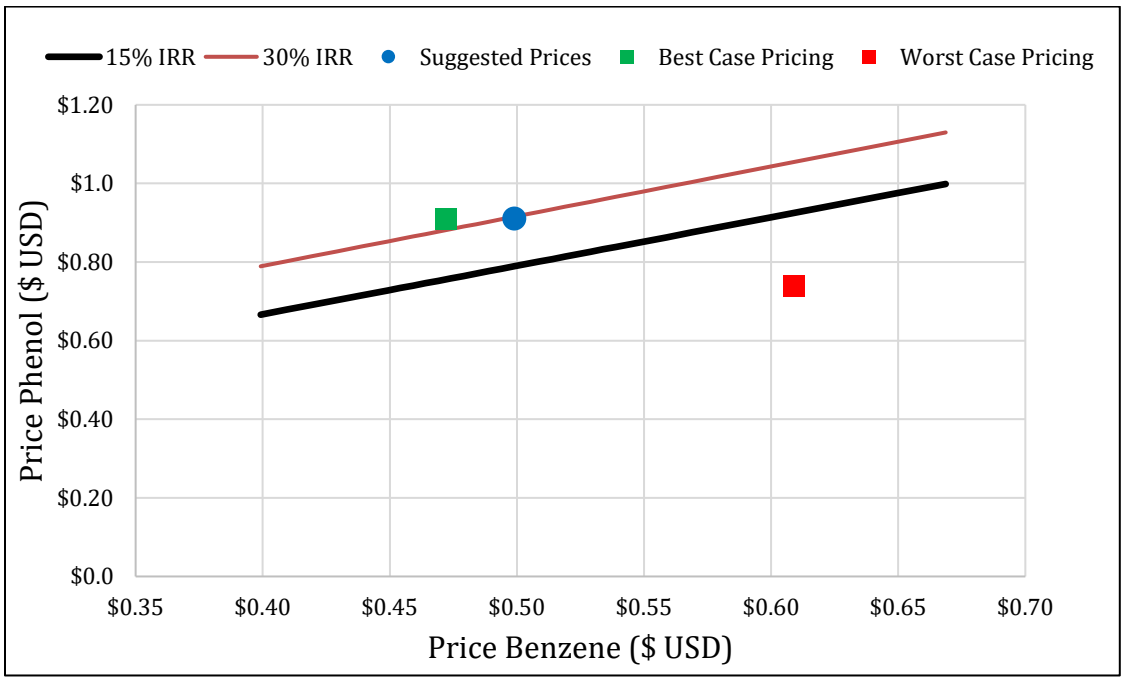


Figure 20.5. Phenol and benzene market pricing required to maintain a 15% and 30% project IRR over a fifteen-year lifespan. Variations in chemical pricing from our marketing team allows us to weigh the profitability of our process in light of realistic market data.

This figure illustrates pricing requirements to generate both a 15% and 30% IRR for the proposed project. Under the assumption that benzene and phenol market prices are aligned with those provided, denoted by the blue point, the project is profitable and generates an IRR of 29.2%, as previously mentioned. The green point indicates the best possible pricing situation, while the red point indicates the worst possible pricing. Our base case process was designed near the best-case scenario. An IRR of 15% could still be achieved even if phenol prices drop by 8% while benzene prices increase by 8%.

However, the margin between phenol and benzene prices is a much more important metric to consider for profitability, as it provides a strong indication of the profit margin for direct benzene to phenol production. Figure 20.6 displays pricing data from NEXANT for these two industrial compounds over the last eleven years.

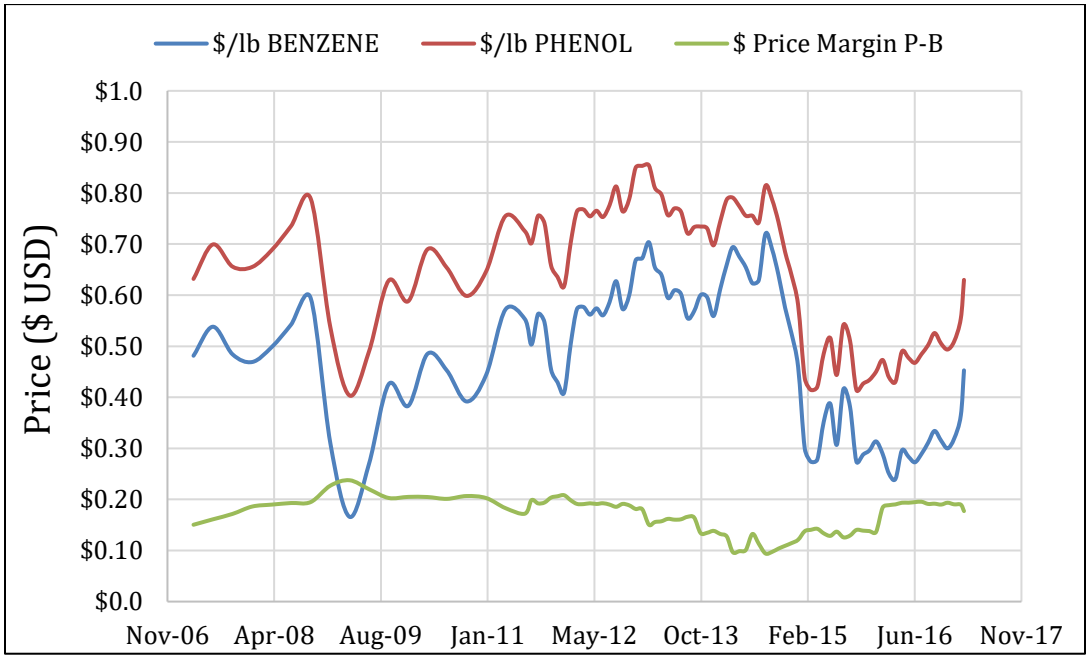


Figure 20.6. Prices and price margin data for benzene and phenol in the U.S. between Nov. 2006 and Feb. 2017 provided by NEXANT. This historical margin has remained relatively constant, indicating a strong correlation between the pricing for the two chemicals.

The market prices for benzene and phenol in the U.S. from Nov. 2006 to Feb. 2017 more realistically contextualize the profitability of this project. The data indicates that assuming benzene pricing of $0.499/lb was certainly reasonable, though a phenol price of $0.91/lb phenol was bullish.

It is possible that the optimistic prices from our company's marketing group are grounded in expectations for a future return to high crude oil prices and a corresponding rise in phenol prices. Phenol shortages are equally as likely, and could drive supply down and prices up if many of the cumene-based production plants shutdown due to unfavorable economics in the propylene to acetone conversion. ICIS predicts U.S. phenol and benzene prices to remain steady in 2017, though there is a possibility for phenol and derivatives like polycarbonate to rebound on increased crude oil production.[20.5] Time alone will tell which forecasts are most probable.

The data indicates that benzene and phenol prices have moved together over time and maintained a price margin between $0.10/lb and $0.20/lb for the last decade. This margin is much less than the $0.41/lb price differential suggested by our marketing team. While we do recommend investment in the process based on data from our marketing team, under the conditions provided by NEXANT, our group does not recommend moving forward. The prices from 2017 indicate unfavorable economics and yield a net loss of $75MM over fifteen years.

The requirement for profitability of this project under the current design is a phenol selling price of $0.79/lb. If prices for phenol rise above this value, we recommend development of the proposed process as a replacement for the Hock process. It is ultimately up to management to make

[20.5] Dietrich, John. "OUTLOOK '17: US Polycarbonate Growth Tied to Economy." *ICIS.com*. ICIS, 23 Dec. 2016. Web. 16 Apr. 2017.

an informed prediction of future raw material and product pricing before conducting further research or beginning plant construction.

Section 21

Other Considerations

Section 21.1: Environmental Considerations

Benzene is one of the main chemical derivatives from crude oil, and although it is used extensively in industry, it is dangerous to humans, animals, and the environment. According to the Safety Data Sheet on liquid benzene issued by Chevron Phillips, the LC50 (50% lethal concentration) for an exposure time of 96 hours for aquatic life is 5.3 ppm. Benzene is also a known carcinogen that should not be released into the environment. Uncontrolled discharge of phenol into the environment is similarly dangerous, as aquatic life will be at risk. A flare system was designed for the non-condensable components, unrecycled benzene, and for collection of all possible leakage points within process units and piping. A benzene storage tank was also designed in the event of pipeline malfunction.

Section 21.2: Safety & Health Considerations

To ensure safe working conditions, OSHA recommends a peak concentration of 50 ppm for benzene and 5 ppm for phenol. Benzene is an immediate danger to life at concentrations above 500 ppm. Benzene and phenol are also flammable. Plant workers will wear flame retardant, antistatic, and chemically impermeable protective gear. A ventilation system will be designed to maintain minimal oxygen concentrations of 19.5% by volume at ambient conditions. Additionally, all workers will be equipped with National Institute of Occupational Safety and Health (NIOSH) approved respirators.

The upper and lower explosion limits of benzene in air are 7.8 and 1.2% by volume, respectively. Phenol's upper and lower explosion limits in air are 1.8 and 8.6% by volume, respectively. Throughout the process, the volume of benzene and phenol relative to air, or oxygen, is kept significantly above their upper explosion limits.

Process safety was also considered for the reactor design. Given extreme operating conditions, the reactor effluent is cooled and depressurized to allow for safer, more ambient downstream operating conditions.

Section 21.3: Process Control Considerations

The implementation of controllers is necessary to maintain the relatively isothermal conditions of the reactors. The potentially variable temperature of the reactor effluent determines the amount of heat exchanged in counter-current heat exchanger E-201. This causes the amount of energy required to pre-heat the reactor feed in E-202 to fluctuate. The hot oil heater E-202 can be modelled as part of a control system. A process controller can be designed to manipulate oil temperature leaving furnace H-001 or the oil flowrate exchanging heat in E-202. Industrial consultants suggested the use of a flow controller. A temperature controller would increase furnace duty to meet the set-point temperature, yet responds slowly compared to an oil flow controller. The use of a flow controller can optimize natural gas fuel flow to the furnace by setting the amount of fuel fed to the furnace as constant. A flow controller may result in greater overshoot of the set-point temperature but is considered inconsequential since this overshoot is likely to remain within the allowable bounds set for reaction temperature increase.

Additional controllers would be used to adjust the inert N_2 pressure in all four of the storage tanks. By manipulating N_2 flowrate, the pressure can be maintained even when filling up or removing large quantities of the stored chemicals. A pressure greater than the vapor pressure of the contents is used to prevent atmospheric discharge.

Section 21.4: Plant Location, Layout, Start Up

The proposed plant will be located on the U.S. Gulf Coast as part of an industrial chemical complex. Prior to plant start-up, considerations for plant layout need to ensure worker and environmental safety. This would include positioning the reaction process section within a containment vessel in a remote part of the plant in case of accidental explosions. The plant also needs to meet all state and federal regulations. Preliminary costs, as determined in Section 18, pg. 114, include site preparation, service facilities, land cost, and contractor fees. Site preparation requires $7.8MM, service facilities $1.9MM, cost of land $1.1MM, and contractor fees of $8.7MM.

Plant start-up, including the loading of chemicals into their respective process vessels, costs $5.7MM. Costs obtained using *Seider et. al, 2017* may be below the actual price due to the approximate nature of the recommended percentages.

Section 22

Conclusions and Recommendations

Thorough analysis of the proposed design indicates that the direct process to produce phenol from benzene developed by researchers at CSIR warrants further investigation. In accordance with the project objective, the process produces 500MM lb of liquid phenol per year. Economic analysis estimates an NPV of $90MM with an IRR of 29.2%. Prior to further development of the process, design calculations, as seen in Appendix 4, pg. 211, should be revisited to confirm their accuracy or to adjust assumptions. The calculated capital and operating costs may be an underestimate, as the design is not fully refined.

Additional optimization of the process is possible with the development of a kinetic model. The CSIR patent provides limited kinetic data but with the help of a comprehensive kinetic model, reactor conditions can be further adjusted to achieve desired conversion and selectivity. Patent data must first be confirmed prior to the development of such a model.

Limited catalyst data is included in the patent; assumptions are made for the catalyst density, activity, longevity, and price. Research into the copper-chromium catalyst will result in a more accurate design.

The reactor contains four segments with intercoolers to keep temperature and pressure close to 662 °F and 580 psig, with conversion assumed to be equivalent throughout each section. In the design of the reactor, an allowable temperature fluctuation of 54 °F per segment was assumed possible without having a significant effect on conversion and selectivity. Should further research refute this assumption, the reactor will have to be re-designed.

The profitability of the proposed design depends heavily on the market price of benzene and phenol. According to our marketing team, phenol is valued at $0.91/lb. Sensitivity analyses revealed that a minimum requirement for profitability of this project under the current design is a phenol selling price of $0.79/lb. Historical NEXANT market data for phenol and benzene, as

discussed in Section 20.1, pg. 132, indicate a price margin of about $0.20/lb for the last decade. This margin is 50% less than the $0.41/lb price differential suggested by our marketing team, and yields a net loss of $75MM over fifteen years. Ultimately, we do recommend investment in this project based on data provided from our marketing team in the proposal. However, in light of realistic cost information, we advise caution before proceeding with any investment.

Section 23

Acknowledgements

Our team would like to express our gratitude for the constant support and advice afforded by Dr. Holleran and Mr. Vrana. Dr. Holleran provided tremendous guidance in our analysis of the impact that the amount of unreacted benzene recovered has on our project. He consistently gave us recommendations in considering some of the most important process variables. We are extremely grateful that Professor Vrana was constantly available for meetings, questioning, and any type of discussion. Their guidance and recommendations greatly aided us with the development of our process and helped us to meet deadlines for deliverables.

We would like to thank the industrial consultants who attended our design meetings and offered advice: Mr. Gary Sawyer of CDI Corp., Mr. Stephen Tieri of DuPont, Dr. Michael Grady of Axalta, Dr. Gopalratnam, Dr. Bockrath, and Mr. David Kolesar of Dow Chemical, and Professor Leonard Fabiano. Their insight was valuable, especially with regards to safety, and provided useful design considerations. Special thanks are given to Mr. Gary Sawyer for guiding us in the right direction in the development of a thorough profitability analysis.

Our group would especially like to extend our fullest appreciation towards Professor Fabiano, who worked closely with us throughout the semester. Professor Fabiano's expertise with ASPEN, heat exchanger design, and distillation column design taught us a great deal about the chemicals processing industry, and allowed for an extremely thorough process design that would not have been possible otherwise. Thank you for the privilege of your time.

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Section 25

Appendices

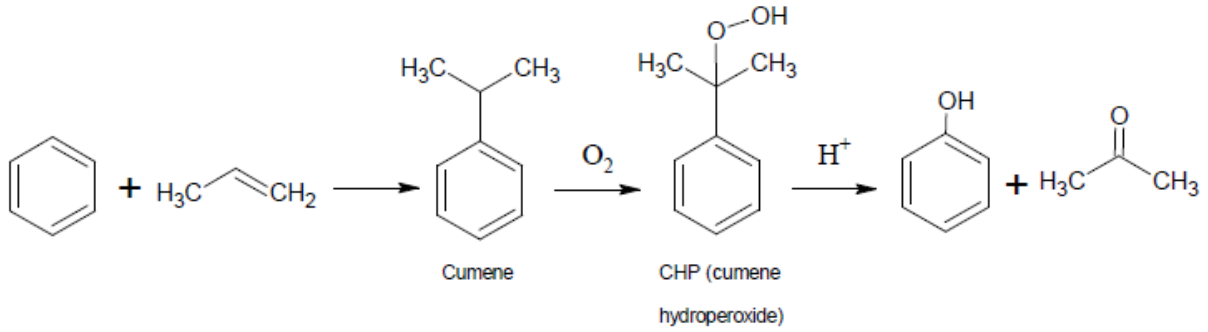
Appendix 1

Project Prompt

3. Direct Route to Phenol From Benzene
(recommended by Bruce M. Vrana, DuPont)

Phenol is a major chemical intermediate used in a variety of other products. Phenolic resins are used in a wide range of products, including printed circuit boards. Phenol is a raw material to make polycarbonate, used in CD, DVD and Blu-ray discs. Phenol can be converted to caprolactam and ultimately nylon-6, or to adipic acid and ultimately nylon-6,6, both used for fibers and engineering polymers. There are a wide variety of other applications for this versatile intermediate.

Phenol is conventionally made from cumene using the following chemistry:



This route has several drawbacks. Growth in demand for propylene has exceeded the growth in supply, driving propylene prices higher. Also, one mole of acetone is made per mole of phenol. The acetone must be sold at a reasonable price in order to have favorable economics on making the phenol. Although acetone has numerous uses, phenol producers often have difficulty selling the byproduct at an attractive price. Effectively, this process converts high value propylene into low value acetone. In fact, although you could sell more phenol, your company has decided to not expand phenol capacity if it produces acetone as a coproduct.

A team of scientists at the Council of Scientific and Industrial Research (CSIR) in New Delhi has recently patented a direct process from benzene to phenol. Their vapor-phase process uses air to oxidize benzene directly over a supported copper-chromium catalyst with about 95% yield at 28% conversion of benzene.

Your company is considering licensing this technology. Your team has been assembled to determine whether the process will be economical before engaging in any discussions with CSIR. Because these negotiations can be sensitive, your management has forbidden any form of contact with anyone at CSIR during your design. You may use only information that you can find in the public domain, in the patent, on the Internet, etc. The objective is to obtain a license at the lowest possible price, so you do not want to tip off your company's interest in the process until your engineering analysis is complete.

Based on data in the patent, design the optimum process to make 500MM lb/yr of phenol from benzene at your plant complex on the U.S. Gulf Coast. You will need to focus on the process to make phenol, not the process to make the catalyst, which you can assume will be produced for

you by a catalyst vendor. Benzene is available on site for $1,100/metric ton. Phenol is worth $2,000/metric ton to your company. All prices are forecasts by your marketing organization for long term average prices, expressed in 2017 dollars.

You will need to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before approaching CSIR to discuss a license. Test your economics to reasonable ranges of your assumptions. If there are any possible "showstoppers" (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

The plant design should be as environmentally friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Remember that if the negotiations are successful, you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference

U. S. Patent 8,772,552, July 8, 2014, assigned to Council of Scientific and Industrial Research.

Appendix 2

Project Patent

US008772552B2

(12) **United States Patent**
Bal et al.

(10) **Patent No.: US 8,772,552 B2**
(45) **Date of Patent: Jul. 8, 2014**

(54) **PROCESS FOR THE SELECTIVE HYDROXYLATION OF BENZENE WITH MOLECULAR OXYGEN**

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(73) Assignee: **Council of Scientific & Industrial Research**, New Delhi (IN)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

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(52) **U.S. Cl.**
USPC **568/802**; 502/317; 502/305

(58) **Field of Classification Search**
USPC 568/802; 502/317, 305
See application file for complete search history.

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Primary Examiner — Johann R Richter
Assistant Examiner — Mark Luderer
(74) *Attorney, Agent, or Firm* — Blank Rome LLP

(57) **ABSTRACT**

The present invention provides an improved process for the selective hydroxylation of benzene. The process provides a direct single step selective vapor phase hydroxylation of benzene to phenol using molecular oxygen (air) over Cu—Cr oxide catalysts. The process provides benzene conversion of 10 to 45% and selectivity for phenol up to 100%.

9 Claims, No Drawings

PROCESS FOR THE SELECTIVE HYDROXYLATION OF BENZENE WITH MOLECULAR OXYGEN

FIELD OF INVENTION

The present invention relates to an improved process for the selective hydroxylation of benzene with molecular oxygen (air) over solid catalysts. More particularly, the present invention relates to an improved process for the vapour phase selective hydroxylation of benzene to phenol by using molecular oxygen (air) over Cu—Cr oxide.

BACKGROUND OF THE INVENTION

Phenol is a very important chemical for the chemical industry due to its widespread use in the fields of resin, plastics, pharmaceuticals, agrochemicals, etc. It is mainly used for the production of a large no of intermediates such as bisphenol, caprolactum, aniline, alkylphenol, chlorophenol, salicylic acid, etc., which are then further used to produce epoxy resin for paints, polycarbonate plastics for CDs and domestic appliances, nylon, polyamides, antioxidants, surfactants, detergents, anticeptics, medicines etc. At present phenol is mainly produced by three steps Cumene Process. However, the process has several disadvantages such as poor ecology, formation of an explosive intermediates (cumene hydroperoxide), multistep character which makes it difficult to achieve high phenol yield w.r.t. benzene. The main concern in the fine chemical and drug intermediates are the amount of waste generated per unit weight of desired product (called E-factor by R A Sheldon in Chemsitry & Industry, 6 Jan. 1997, P 13) and poor atom efficiencies (kg of product produced per Kg of reactants used) due to the use of stoichiometric reagents and minerals acid/base catalysts. In this context, the use of solid catalysts which are eco-safe and reusuable become important. Moreover a major problem with this process is that it produces phenol is driving its price down and also hurting the economics of phenol as well. This concern is the impetus for researchers to develop a direct single step co-product free and environment friendly route to phenol.

There are reports on the production of phenol by direct hydroxylation of benzene with different oxidants over different solid catalyst but to the best of our knowledge there is no reference for the use of molecular oxygen (air) only for this purpose.

Reference may be made to article in the Journal of Physical Chemistry, 1983, 87, 903-905, in which Japanese workers reported the use of nitrous oxide for the hydroxylation of benzene to phenol—using vanadium pentaoxide/silica catalyst at 550° C. to achieve 10% benzene conversion and 70% phenol selectivity.

Reference may also be made to patents WO9527691, 1995 and WO9527560, 1995 wherein Panov et al developed a one step process for the manufacture of phenol from benzene using nitrous oxide as the and ZSM-5 and ZSM-11 as the catalysts. The drawbacks of this process are deactivation of catalyst, loss of selectivity of catalyst and side reaction (combustion of benzene by nitrous oxide). It is economically attractive only if N_2O is available as the by product of some other process such as the two step oxidation of cyclohexane to adipic acid.

Reference may be made to article in J. Chem. Soc. Chem. Com., 1992, 1446-1447 wherein Tatsumi et al. describe a process for the preparation of phenol from benzene with H_2 and O_2 which uses a catalyst consisting of palladium supported on TS-1. Operating according to this process, a conversion of benzene of 0.07% is obtained with a turnover of Palladium of 13.5.

Another reference may be made to European patent EP0894783, 1998, wherein a process for the synthesis of phenol by catalytic oxidation of benzene in the presence of titanium silicate and by H_2O_2 prepared in situ by reaction of oxygen carbon monoxide and water in the presence of catalytic complexes consisting of palladium with a nitrogenated ligand and a non-coordinating counter ion. The selectivity of benzene to phenol is greater than 95%, but benzene conversions were only 1-2%.

Reference may be made to the article in Journal of Molecular CatalysisA: Chemical 2006, 253, 1-7, wherein phenol is prepared by homogeneous liquid phase direct catalytic oxidation of benzene at room temperature in acetonitrile solvent using sodium metavenadate as the catalyst and hydrogen peroxide as the oxidant. Phenol yield of 13.5% with a selectivity of 94% was reported.

Reference may be made to Ind. Eng. Chem. Res. 1999, 38, 1893-1903, wherein phenol was synthesized by direct liquid phase benzene hydroxylation by H_2O_2 using V-MCM-41 as the catalyst under mild conditions. Operating accordingly to this process, a conversion of benzene of 13% and selectivity for phenol of 48% was obtained.

Another reference may be made to Science 2002, 105, 295, wherein phenol was obtained by direct vapour phase hydroxylation of benzene using Pd-membrane as a catalyst using O_2 and H_2 as the oxidant. Phenol yield of 12% and selectivity of 80-97% was obtained.

Another reference may be made to article in Applied Clay Science 2006, 33, 1-6, wherein selective direct hydroxylation of benzene with hydrogenperoxide to phenol was carried out on a clay-supported vanadium oxide catalyst. Under mild reaction conditions at 60° C., high selectivity to phenol of 94% was obtained but conversion of benzene was only 14%.

Another reference may be made to article Angew. Chem. Int. Ed. 2006, 45, 448, wherein phenol was obtained by direct vapour phase hydroxylation of benzene using Re cluster/zeolite as a catalyst using O_2 and NH_3 as the oxidant. Phenol yield of 5% and selectivity of 80-97% was obtained.

The drawback of the processes reported so far is that they do not exhibit sufficiently high conversions of benzene for high selectivity of phenol to be of interest for industrial application. In most of the cases hazardous oxidizing agent N_2O, H_2O_2 or expensive H_2 with O_2 or reducing agent NH_3 with O_2 was used and also lots of unnecessary by-products was formed. In addition, the catalysts used have a limited activity under the operating conditions. There is, therefore, an evident necessity for further improvements in the process for the selective conversion of benzene to phenol.

OBJECTIVES OF THE INVENTION

The main object of the present invention is to provide an improved process for the selective hydroxylation of benzene with molecular oxygen (air) over solid catalysts which obviates the drawbacks of hitherto known methods as detailed above.

Another object of the present invention is to provide an improved process for the selective hydroxylation of benzene with molecular oxygen (air) as the oxidant and Cu—Cr oxide as the catalyst.

Still another object of the present invention is to provide an improved process, which gives phenol from benzene with high selectivity.

Yet another object of the present invention is to provide a process which uses environmental friendly green oxidizing agent, air for the synthesis of phenol.

Yet another object of the present invention is to provide a process which works under continuous process for the synthesis of phenol.

Yet another object of the present invention is to provide a process which works under mild conditions for the synthesis of phenol.

SUMMARY OF THE INVENTION

Accordingly, the present invention provides an improved process for the selective hydroxylation of benzene with molecular oxygen (air) over solid catalysts which comprises reacting benzene with air in the pressure range of 1-5 MPa, at a temperature of 150-450° C. with a liquid hourly space velocity (LHSV, benzene feed/g catalyst/hour) in the range of 20 to 400 for a period of 1-30 hrs in the presence of Cu—Cr oxide catalyst to obtain phenol.

In an embodiment of the invention, the molar ratio of Cu to Cr of the catalyst varied in the range of 0.1 to 0.5.

In one embodiment of the invention, the air pressure is preferably in the range of 2-5 MPa.

In another embodiment of the invention, the reaction temperature is preferably in the range 200-400° C.

In yet another embodiment, the liquid hourly space velocity (LHSV) is preferably in the range 30 to 300.

In still another embodiment, the reaction time used is preferably in the range 2-30 h.

In still another embodiment, the conversion of benzene is in the range of 1-42%.

In still another embodiment, the selectivity of the phenol obtained in the range of 50-100%.

In still another embodiment, yield of phenol is in the range of 2-30%.

DETAILED DESCRIPTION OF THE INVENTION

The present invention provides an improved process for the production of phenol by vapour phase selective hydroxylation of benzene using air as the oxidant and Cu—Cr oxide as the catalyst which involves the following steps

1. Synthesis of Cu—Cr oxide using the gel composition of $Cu(NO_3)_2$, $Cr(NO_3)_3$, cetyltrimethylammonium bromide, hydrazine, in the molar ratio of Cu: CTAB: Hydrazine: H_2O=1:0.75:1:300
   40 g $Cr(NO_3)_3.9H_2O$ was dissolved in 40 g water and 2.95 g $Cu(NO_3)_2.3H_2O$ was added to it. Into this solution, 3.9 g cetyltrimethylammonium bromide dissolved with 5 g H_2O was added dropwise to get a homogeneous mixture. Then 0.5 g hydrazine dissolved with 2 g water was added dropwise to this mixture. The gel formed was stirred for 3 h and finally the mixture was hydrothermally treated at 140-170° C. for 20-24 h in a Teflon lined stainless steel autoclave under a autogeneous pressure. The product was washed with excess distilled water and ethanol and dried at ambient temperature for 6 -10 h and calcined in the temperature between 300 to 550° C. in air.
2. The molar ratio of Cu to Cr varied in the range between 0.1 to 0.7
3. Calcination of the materials at 300-750° C. for 4-8 h
4. Benzene hydroxylation was carried out in a fixed bed down-flow reactor using benzene and air as feeds for 1 to 30 h to get phenol.
   The air pressure is preferably in the range 2 to 5 MPa
   The reaction temperature is preferably in the range 200-400° C.
   The liquid hourly space velocity (LHSV) is preferably in the range 30 to 300
   The benzene conversion is obtained 10-30 wt % and selectivity to phenol approaching 100%.
   The detailed steps of the process are:
   The reaction was carried out in a fixed bed down flow high pressure reactor by charging 0.2 g catalyst. The pressure of the reactor was maintained by using air.
   Benzene was introduced in the reactor by using a HPLC pump. The reaction mixtures were analyzed by two online GCs with an FID detector by using capillary column for hydrocarbons and a TCD detector by using a Porapack-Q column for inorganic materials online GC

The following examples are given by way of illustration of working of the invention in actual practice and should not be constructed to limit the scope of the present invention in any way.

EXAMPLE—1

This example describes the hydroxylation of benzene by vapour phase reaction in air using Cu—Cr oxide as the catalyst.

Process Conditions
Catalyst: 0.2 g
Cu:Cr molar ratio in the catalyst=1:2.5
Air pressure : 4 Mpa
Benzene flow=0.1 ml/min (LHSV=30)
Temperature: 350° C.
Reaction time: 6 h
Product Analysis:
Benzene conversion: 28.9%
Selectivity of phenol : 95.2%

EXAMPLE—2

The example describes the effect of temperature on yield and selectivity of phenol. The product analysis presented in Table—1.

Process Conditions:
Catalyst: 0.2 g
Cu:Cr molar ratio in the catalyst=1:2.5
Air pressure : 4 Mpa
Benzene flow=0.1 ml/min
Reaction time: 6 h

TABLE 1

Effect of temperature on benzene conversion, phenol yield and selectivity

Temperature	Benzene Conversion	Phenol	
(° C.)	(%)	Yield	Selectivity
200	2.4	2.4	100
250	7.5	7.4	98.4
300	17.4	16.9	97.2
350	28.9	27.5	95.2
400	41.7	21.1	50.7

EXAMPLE—3

The example describes the effect of time on stream on yield and selectivity of phenol. The product analysis presented in Table 2

Process Conditions:
Catalyst: 0.2 g
Cu:Cr molar ratio in the catalyst=1:2.5
Air pressure : 4 Mpa
Benzene flow=0.1 ml/min
Reaction temperature : 350° C.

TABLE 2

Effect of time on stream on benzene conversion, phenol yield and selectivity

Time on stream	Benzene Conversion	Phenol	
(h)	(%)	Yield	Selectivity
2	28.2	27.5	95.2
6	28.9	27.5	95.1
12	29.4	28.1	95.6
18	28.5	27.4	96
28	27.9	26.5	94.9

EXAMPLE—4

The example describes the effect of air pressure on yield and selectivity of phenol. The product analysis presented in Table—3.
Process Conditions:
Catalyst: 0.2 g
Cu:Cr molar ratio in the catalyst=1:2.5
Reaction temperature : 350° C.
Benzene flow=0.1 ml/min
Reaction time: 6 h

TABLE 3

Effect of air pressure on benzene conversion, phenol yield and selectivity

Reaction Pressure	Benzene Conversion	Phenol	
(MPa)	(%)	Yield	Selectivity
2	2.5	2.1	97.1
3	17.4	16.7	95.8
4	28.9	27.5	95.1
5	31.3	24.9	79.5

EXAMPLE—5

The example describes the effect of liquid hourly space velocity on yield and selectivity of phenol. The product analysis presented in Table—4.
Process Conditions:
Catalyst: 0.2 g
Cu:Cr molar ratio in the catalyst=1:2.5
Reaction temperature : 350° C.
Air pressure: 4 MPa
Reaction time: 6 h

TABLE 4

Effect of liquid hourly space velocity (LHSV) on benzene conversion, phenol yield and selectivity

LHSV	Benzene	Phenol	
(ml benzene/h/g_{cat})	Conversion (%)	Yield	Selectivity
30	28.9	27.5	95.1
60	20.1	19.3	96.2
100	12.5	12.1	96.7
300	4.6	4.5	97.1

The main advantages of the present invention are:

1. The process of the present invention converts benzene to phenol in a single step with a single catalyst.
2. The process provides not only good conversion but also good selectivity for phenol.
3. The oxidizing agent, air, used in this process has the major advantages of this process.
4. The process does not produce any by-products is also a major advantage of this process.
5. The process does not need any addition reagent to generate active oxygen.
6. The catalyst is used in very low amounts.
7. The catalyst does not deactivate till 30 h with the reaction stream.

We claim:

1. A process for making phenol comprising the step of selectively hydroxylating benzene with molecular oxygen over solid catalysts which comprises reacting benzene with air in the pressure range of 1-5 MPa, at a temperature of 150-450° C. with a liquid hourly space velocity (LHSV, benzene feed/g catalyst/hour) in the range of 20 to 400 for a period of 1-30 hrs to obtain phenol, wherein the solid catalyst is Cu—Cr oxide.

2. A process as claimed in claim **1**, wherein the molar ratio of Cu to Cr of the catalyst varied in the range of 0.1 to 0.5.

3. A process as claimed in claim **1**, wherein the air pressure is in the range of 2-5 MPa.

4. A process according to claim **1**, wherein the reaction temperature is in the range 200-400° C.

5. A process as claimed in claim **1**, wherein the liquid hourly space velocity (LHSV) is in the range 30 to 300.

6. A process as claimed in claim **1**, wherein the reaction time used is in the range 2-30 h.

7. A process as claimed in claim **1**, wherein the conversion of benzene is in the range of 1-42%.

8. A process as claimed in claim **1**, wherein the selectivity of the phenol obtained in the range of 50-100%.

9. A process as claimed in claim **1**, wherein the molecular oxygen is provided from air.

* * * * *

Appendix 3

Safety Data Sheets

SAFETY DATA SHEET

Benzene

Version 1.9 Revision Date 2016-01-08

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product information

Product Name : Benzene
Material : 1098293, 1059192, 1059060, 1037212, 1037213, 1037103, 1029170, 1037104, 1015526, 1016960

Company : Chevron Phillips Chemical Company LP
10001 Six Pines Drive
The Woodlands, TX 77380

Emergency telephone:

Health:
866.442.9628 (North America)
1.832.813.4984 (International)
Transport:
CHEMTREC 1.800.424.9300 (within USA and Canada) or 703.527.3887 (outside USA and Canada)
Asia: +800 CHEMCALL (+800 2436 2255) China:+86-21-22157316
EUROPE: BIG +32.14.584545 (phone) or +32.14583516 (telefax)
South America SOS-Cotec Inside Brazil: 0800.111.767 Outside Brazil: +55.19.3467.1600

Responsible Department : Product Safety and Toxicology Group
E-mail address : SDS@CPChem.com
Website : www.CPChem.com

SECTION 2: Hazards identification

Classification of the substance or mixture
This product has been classified in accordance with the hazard communication standard 29 CFR 1910.1200; the SDS and labels contain all the information as required by the standard.

Emergency Overview

Danger

Physical state: Liquid **Color**: Clear, Colorless **Odor**: sweet, distinct

OSHA Hazards : Flammable Liquid, Aspiration hazard, Carcinogen, Moderate skin irritant, Moderate eye irritant, Mutagen, Target Organ Effects

Classification

SAFETY DATA SHEET

Benzene

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: Flammable liquids , Category 2
Skin irritation , Category 2
Eye irritation , Category 2A
Germ cell mutagenicity , Category 1B
Carcinogenicity , Category 1A
Specific target organ systemic toxicity - repeated exposure , Category 1 , Blood
Aspiration hazard , Category 1

Labeling

Symbol(s) :

Signal Word : Danger

Hazard Statements : H225: Highly flammable liquid and vapor.
H304: May be fatal if swallowed and enters airways.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H340: May cause genetic defects.
H350: May cause cancer.
H372: Causes damage to organs (Blood) through prolonged or repeated exposure.

Precautionary Statements : **Prevention:**
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.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P260 Do not breathe dust/fume/gas/mist/vapor/spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/ eye protection/ face protection.
P281 Use personal protective equipment as required.
Response:
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P331 Do NOT induce vomiting.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/

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attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
Storage:
P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
Disposal:
P501 Dispose of contents/ container to an approved waste disposal plant.

Carcinogenicity:

IARC	Group 1: Carcinogenic to humans	
	Benzene	71-43-2
NTP	Known to be human carcinogen	
	Benzene	71-43-2
ACGIH	Confirmed human carcinogen	
	Benzene	71-43-2

SECTION 3: Composition/information on ingredients

Synonyms : Aromatic Benzene
Benzol
Cyclohexatriene
Phene
Phenyl Hydride

Molecular formula : C6H6

Component	CAS-No.	Weight %
Benzene	71-43-2	100

SECTION 4: First aid measures

General advice : Move out of dangerous area. Show this material safety data sheet to the doctor in attendance. Material may produce a serious, potentially fatal pneumonia if swallowed or vomited.

If inhaled : If unconscious place in recovery position and seek medical advice. If symptoms persist, call a physician.

In case of skin contact : If skin irritation persists, call a physician. If on skin, rinse well with water. If on clothes, remove clothes.

In case of eye contact : Immediately flush eye(s) with plenty of water. Remove contact lenses. Protect unharmed eye. Keep eye wide open while rinsing. If eye irritation persists, consult a specialist.

If swallowed : Keep respiratory tract clear. Never give anything by mouth to an unconscious person. If symptoms persist, call a physician.

Take victim immediately to hospital.

SECTION 5: Firefighting measures

Flash point	:	-11 °C (12 °F) Method: Tag closed cup
Autoignition temperature	:	498 °C (928 °F)
Suitable extinguishing media	:	Alcohol-resistant foam. Carbon dioxide (CO_2). Dry chemical.
Unsuitable extinguishing media	:	High volume water jet.
Specific hazards during fire fighting	:	Do not allow run-off from fire fighting to enter drains or water courses.
Special protective equipment for fire-fighters	:	Wear self-contained breathing apparatus for firefighting if necessary.
Further information	:	Collect contaminated fire extinguishing water separately. This must not be discharged into drains. Fire residues and contaminated fire extinguishing water must be disposed of in accordance with local regulations. For safety reasons in case of fire, cans should be stored separately in closed containments. Use a water spray to cool fully closed containers.
Fire and explosion protection	:	Do not spray on an open flame or any other incandescent material. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapors). Use only explosion-proof equipment. Keep away from open flames, hot surfaces and sources of ignition.
Hazardous decomposition products	:	No data available.

SECTION 6: Accidental release measures

Personal precautions	:	Use personal protective equipment. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
Environmental precautions	:	Prevent product from entering drains. Prevent further leakage or spillage if safe to do so. If the product contaminates rivers and lakes or drains inform respective authorities.
Methods for cleaning up	:	Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

SAFETY DATA SHEET

Benzene

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SECTION 7: Handling and storage

Handling

Advice on safe handling	:	Avoid formation of aerosol. Do not breathe vapors/dust. Avoid exposure - obtain special instructions before use. Avoid contact with skin and eyes. For personal protection see section 8. Smoking, eating and drinking should be prohibited in the application area. Provide sufficient air exchange and/or exhaust in work rooms. Container may be opened only under exhaust ventilation hood. Open drum carefully as content may be under pressure. Dispose of rinse water in accordance with local and national regulations. Electrostatic charge may accumulate and create a hazardous condition when handling this material. To minimize this hazard, bonding and grounding may be necessary, but may not by themselves be sufficient. Review all operations, which have the potential to generating and accumulation of electrostatic charge and/or a flammable atmosphere (including tank and container filling, splash filling, tank cleaning, sampling, gauging, switch loading, filtering, mixing, agitation, and vacuum truck operations) and use appropriate mitigating procedures. For more information, refer to OSHA Standard 29 CFR 1910.106 "Flammable and Combustible Liquids"; National Fire Protection Association (NFPA 77), "Recommended Practice on Static Electricity"; and/or the American Petroleum Institute (API) Recommended Practice 2003, "Protection Against Ignitions Arising Out of Static, Lightning, and stray Currents". Avoid formation of aerosol. Do not breathe vapors/dust. Avoid exposure - obtain special instructions before use. Avoid contact with skin and eyes. For personal protection see section 8. Smoking, eating and drinking should be prohibited in the application area. Take precautionary measures against static discharges. Provide sufficient air exchange and/or exhaust in work rooms. Container may be opened only under exhaust ventilation hood. Open drum carefully as content may be under pressure. Dispose of rinse water in accordance with local and national regulations.
Advice on protection against fire and explosion	:	Do not spray on an open flame or any other incandescent material. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapors). Use only explosion-proof equipment. Keep away from open flames, hot surfaces and sources of ignition.

Storage

Requirements for storage areas and containers	:	No smoking. 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. Observe label precautions. Electrical installations / working materials must comply with the technological safety standards.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

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Benzene

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US

Ingredients	Basis	Value	Control parameters	Note
Benzene	ACGIH	TWA	0.5 ppm,	BEI, A1, Skin,
	ACGIH	STEL	2.5 ppm,	BEI, A1, Skin,
	OSHA Z-1-A	TWA	1 ppm,	
	OSHA Z-1-A	CEIL	5 ppm,	
	OSHA Z-2	Peak	50 ppm,	(a),
	OSHA 29 CFR 1910.1028(c)	TWA	1 ppm,	
	OSHA 29 CFR 1910.1028(c)	STEL	5 ppm,	
	OSHA CARC	PEL	1 ppm,	
	OSHA CARC	STEL	5 ppm,	

(a) This standard applies to the industry segments exempt from the 1 ppm 8-hour TWA and 5 ppm STEL of the benzene standard at 1910.1028.
A1 Confirmed human carcinogen
BEI Substances for which there is a Biological Exposure Index or Indices (see BEI® section)
Skin Danger of cutaneous absorption

Immediately Dangerous to Life or Health Concentrations (IDLH)

Substance name	CAS-No.	Control parameters	Update
Benzene	71-43-2	Immediately Dangerous to Life or Health Concentration Value 500 ppm	1995-03-01

Engineering measures

Adequate ventilation to control airborned concentrations below the exposure guidelines/limits. Consider the potential hazards of this material (see Section 2), applicable exposure limits, job activities, and other substances in the work place when designing engineering controls and selecting personal protective equipment. If engineering controls or work practices are not adequate to prevent exposure to harmful levels of this material, the personal protective equipment listed below is recommended. The user should read and understand all instructions and limitations supplied with the equipment since protection is usually provided for a limited time or under certain circumstances.

Personal protective equipment

Respiratory protection : Wear a supplied-air NIOSH approved respirator unless ventilation or other engineering controls are adequate to maintain minimal oxygen content of 19.5% by volume under normal atmospheric pressure. Wear a NIOSH approved respirator that provides protection when working with this material if exposure to harmful levels of airborne material may occur, such as:. Air-Purifying Respirator for Organic Vapors. Use a positive pressure, air-supplying respirator if there is potential for uncontrolled release, exposure levels are not known, or other circumstances where air-purifying respirators may not provide adequate protection.

Hand protection : The suitability for a specific workplace should be discussed with the producers of the protective gloves. Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. Also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion, and the contact time. Gloves should be discarded and replaced if there is any indication of degradation or chemical breakthrough.

Eye protection : Eye wash bottle with pure water. Tightly fitting safety goggles.

Skin and body protection : Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. Wear as appropriate:. Flame retardant

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antistatic protective clothing. Workers should wear antistatic footwear.

Hygiene measures : When using do not eat or drink. When using do not smoke. Wash hands before breaks and at the end of workday.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

Appearance

Physical state	:	Liquid
Color	:	Clear, Colorless
Odor	:	sweet, distinct

Safety data

Flash point	:	-11 °C (12 °F) Method: Tag closed cup
Lower explosion limit	:	1.2 %(V)
Upper explosion limit	:	7.8 %(V)
Oxidizing properties	:	no
Autoignition temperature	:	498 °C (928 °F)
Molecular formula	:	C6H6
Molecular weight	:	78.12 g/mol
pH	:	Not applicable
Pour point	:	No data available
Boiling point/boiling range	:	80 °C (176 °F)
Vapor pressure	:	75.00 MMHG at 20 °C (68 °F)
Relative density	:	0.88 at 25 °C (77 °F)
Water solubility	:	1.88 g/l at 23.5 °C (74.3 °F)
Partition coefficient: n-octanol/water	:	log Pow: 2.13
Relative vapor density	:	2.77 (Air = 1.0)
Evaporation rate	:	2.8
Percent volatile	:	> 99 %

Other information

Conductivity	: < 50 pSm at 20 °C

SECTION 10: Stability and reactivity

Reactivity	: No decomposition if stored and applied as directed.
Chemical stability	: This material is considered stable under normal ambient and anticipated storage and handling conditions of temperature and pressure. No decomposition if stored and applied as directed.

Possibility of hazardous reactions

Conditions to avoid	: Heat, flames and sparks.
Materials to avoid	: May react with oxygen and strong oxidizing agents, such as chlorates, nitrates, peroxides, etc.
Hazardous decomposition products	: No data available
Other data	: No decomposition if stored and applied as directed.

SECTION 11: Toxicological information

Acute oral toxicity

Benzene	: LD50: > 2,000 mg/kg Species: Rat Sex: female

Acute inhalation toxicity

Benzene	: LC50: 44.5 mg/l Exposure time: 4 h Species: Rat Sex: Not Specified Test atmosphere: vapor

Acute dermal toxicity

Benzene	: LD50: > 8,260 mg/kg Species: Rabbit

Benzene
Skin irritation : May cause skin irritation in susceptible persons.

Benzene
Eye irritation : May cause irreversible eye damage.

Sensitization

Benzene : Did not cause sensitization on laboratory animals.

Repeated dose toxicity

Benzene : Species: Rat, female
Sex: female
Application Route: oral gavage
Dose: 0, 25, 50, 100 mg/kg
Exposure time: 103 wk
Number of exposures: 5 d/wk
NOEL: < 25 mg/kg
Lowest observable effect level: 25 mg/kg

Species: Rat, male
Sex: male
Application Route: oral gavage
Dose: 0, 50, 100, 200 mg/kg
Exposure time: 103 wk
Number of exposures: 5 d/wk
NOEL: < 50 mg/kg
Lowest observable effect level: 50 mg/kg

Species: Mouse
Application Route: oral gavage
Dose: 0, 25, 50,100 mg/kg
Exposure time: 103 wk
NOEL: < 25 mg/kg

Carcinogenicity

Benzene : Species: Rat
Sex: female
Dose: 0, 25, 50, 250 mg/kg
Exposure time: 103 wks
Number of exposures: daily, 5 days/week
Test substance: yes
Remarks: zymbal gland carcinomas, squamous cell papillomas

Species: Rat
Sex: male
Dose: 0, 50, 100, 200 mg/kg
Exposure time: 103 wks
Number of exposures: daily, 5 days/week
Test substance: yes
Remarks: zymbal gland carcinomas, squamous cell papillomas

Species: Mouse
Sex: male and female
Dose: 25, 50, 100 mg/kg
Exposure time: 103 wks
Number of exposures: daily, 5 days/week
Test substance: yes
Remarks: Clear evidence of multiple organ carcinogenicity.

Benzene
Aspiration toxicity : May be fatal if swallowed and enters airways.

Substances known to cause human aspiration toxicity hazards or to be regarded as if they cause human aspiration toxicity hazard.

CMR effects

Benzene : Carcinogenicity: Human carcinogen.
Mutagenicity: In vivo tests showed mutagenic effects
Teratogenicity: Did not show teratogenic effects in animal experiments.
Reproductive toxicity: Animal testing did not show any effects on fertility.

Benzene
Further information : Chronic Health Hazard.
Solvents may degrease the skin.

SECTION 12: Ecological information

Toxicity to fish

Benzene : LC50: 5.3 mg/l
Exposure time: 96 h
Species: Oncorhynchus mykiss (rainbow trout)
flow-through test Test substance: yes
Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

Benzene : EC50: 10 mg/l
Exposure time: 48 h
Species: Daphnia magna (Water flea)
static test Test substance: yes
Method: OECD Test Guideline 202

Toxicity to algae

Benzene : ErC50: 100 mg/l
Exposure time: 72 h
Species: Pseudokirchneriella subcapitata (green algae)
Test substance: yes
Method: OECD Test Guideline 201

Elimination information (persistence and degradability)

Biodegradability : This material is expected to be readily biodegradable.

Ecotoxicology Assessment

Acute aquatic toxicity
Benzene : Toxic to aquatic life.

Chronic aquatic toxicity
Benzene : Harmful to aquatic life with long lasting effects.

Results of PBT assessment

Benzene	:	This substance is not considered to be persistent, bioaccumulating and toxic (PBT)., This substance is not considered to be very persistent and very bioaccumulating (vPvB).
Additional ecological information	:	Toxic to aquatic life. An environmental hazard cannot be excluded in the event of unprofessional handling or disposal., Toxic to aquatic life.

SECTION 13: Disposal considerations

The information in this SDS pertains only to the product as shipped.

Use material for its intended purpose or recycle if possible. This material, if it must be discarded, may meet the criteria of a hazardous waste as defined by US EPA under RCRA (40 CFR 261) or other State and local regulations. Measurement of certain physical properties and analysis for regulated components may be necessary to make a correct determination. If this material is classified as a hazardous waste, federal law requires disposal at a licensed hazardous waste disposal facility.

Product	:	The product should not be allowed to enter drains, water courses or the soil. Do not contaminate ponds, waterways or ditches with chemical or used container. Send to a licensed waste management company.
Contaminated packaging	:	Empty remaining contents. Dispose of as unused product. Do not re-use empty containers. Do not burn, or use a cutting torch on, the empty drum.

SECTION 14: Transport information

The shipping descriptions shown here are for bulk shipments only, and may not apply to shipments in non-bulk packages (see regulatory definition).

Consult the appropriate domestic or international mode-specific and quantity-specific Dangerous Goods Regulations for additional shipping description requirements (e.g., technical name or names, etc.) Therefore, the information shown here, may not always agree with the bill of lading shipping description for the material. Flashpoints for the material may vary slightly between the SDS and the bill of lading.

US DOT (UNITED STATES DEPARTMENT OF TRANSPORTATION)
UN1114, BENZENE, 3, II, RQ (BENZENE)

IMO / IMDG (INTERNATIONAL MARITIME DANGEROUS GOODS)
UN1114, BENZENE, 3, II, (-11 °C)

IATA (INTERNATIONAL AIR TRANSPORT ASSOCIATION)
UN1114, BENZENE, 3, II

ADR (AGREEMENT ON DANGEROUS GOODS BY ROAD (EUROPE))

SAFETY DATA SHEET

Benzene

Version 1.9 Revision Date 2016-01-08

UN1114, BENZENE, 3, II, (D/E)

RID (REGULATIONS CONCERNING THE INTERNATIONAL TRANSPORT OF DANGEROUS GOODS (EUROPE))
UN1114, BENZENE, 3, II

ADN (EUROPEAN AGREEMENT CONCERNING THE INTERNATIONAL CARRIAGE OF DANGEROUS GOODS BY INLAND WATERWAYS)
UN1114, BENZENE, 3, II

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Other information	:	**Benzene and mixtures having 10% Benzene or more, S.T. 3, Cat.Y**

SECTION 15: Regulatory information

National legislation

CERCLA Reportable Quantity	:	10 lbs Benzene
SARA 302 Reportable Quantity	:	This material does not contain any components with a SARA 302 RQ.
SARA 302 Threshold Planning Quantity	:	No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.
SARA 304 Reportable Quantity	:	This material does not contain any components with a section 304 EHS RQ.
SARA 313 Ingredients	:	The following components are subject to reporting levels established by SARA Title III, Section 313:
	:	Benzene - 71-43-2

Clean Air Act

Ozone-Depletion Potential	:	This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 12 (40 CFR 61):

SAFETY DATA SHEET

Benzene

Version 1.9 Revision Date 2016-01-08

: Benzene - 71-43-2

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489):

: Benzene - 71-43-2

US State Regulations

Pennsylvania Right To Know

: Benzene - 71-43-2

New Jersey Right To Know

: Benzene - 71-43-2

California Prop. 65 Ingredients : WARNING! This product contains a chemical known in the State of California to cause cancer.

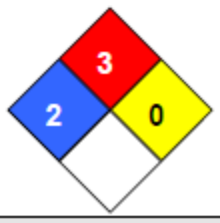
WARNING: This product contains a chemical known in the State of California to cause birth defects or other reproductive harm.

Notification status

Europe REACH	:	On the inventory, or in compliance with the inventory
United States of America TSCA	:	On the inventory, or in compliance with the inventory
Canada DSL	:	On the inventory, or in compliance with the inventory
Australia AICS	:	On the inventory, or in compliance with the inventory
New Zealand NZIoC	:	On the inventory, or in compliance with the inventory
Japan ENCS	:	On the inventory, or in compliance with the inventory
Korea KECI	:	On the inventory, or in compliance with the inventory
Philippines PICCS	:	On the inventory, or in compliance with the inventory
China IECSC	:	On the inventory, or in compliance with the inventory

SECTION 16: Other information

NFPA Classification : Health Hazard: 2
Fire Hazard: 3
Reactivity Hazard: 0



SDS Number:100000068511 13/14

Further information

Legacy SDS Number : CPC00091

Significant changes since the last version are highlighted in the margin. This version replaces all previous versions.

The information in this SDS pertains only to the product as shipped.

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

Key or legend to abbreviations and acronyms used in the safety data sheet			
ACGIH	American Conference of Government Industrial Hygienists	LD50	Lethal Dose 50%
AICS	Australia, Inventory of Chemical Substances	LOAEL	Lowest Observed Adverse Effect Level
DSL	Canada, Domestic Substances List	NFPA	National Fire Protection Agency
NDSL	Canada, Non-Domestic Substances List	NIOSH	National Institute for Occupational Safety & Health
CNS	Central Nervous System	NTP	National Toxicology Program
CAS	Chemical Abstract Service	NZIoC	New Zealand Inventory of Chemicals
EC50	Effective Concentration	NOAEL	No Observable Adverse Effect Level
EC50	Effective Concentration 50%	NOEC	No Observed Effect Concentration
EGEST	EOSCA Generic Exposure Scenario Tool	OSHA	Occupational Safety & Health Administration
EOSCA	European Oilfield Specialty Chemicals Association	PEL	Permissible Exposure Limit
EINECS	European Inventory of Existing Chemical Substances	PICCS	Philippines Inventory of Commercial Chemical Substances
MAK	Germany Maximum Concentration Values	PRNT	Presumed Not Toxic
GHS	Globally Harmonized System	RCRA	Resource Conservation Recovery Act
>=	Greater Than or Equal To	STEL	Short-term Exposure Limit
IC50	Inhibition Concentration 50%	SARA	Superfund Amendments and Reauthorization Act.
IARC	International Agency for Research on Cancer	TLV	Threshold Limit Value
IECSC	Inventory of Existing Chemical Substances in China	TWA	Time Weighted Average
ENCS	Japan, Inventory of Existing and New Chemical Substances	TSCA	Toxic Substance Control Act
KECI	Korea, Existing Chemical Inventory	UVCB	Unknown or Variable Composition, Complex Reaction Products, and Biological Materials
<=	Less Than or Equal To	WHMIS	Workplace Hazardous Materials Information System
LC50	Lethal Concentration 50%		

SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 3.16
Revision Date 05/24/2016
Print Date 03/27/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Phenol

Product Number : 16018
Brand : Sigma-Aldrich

CAS-No. : 108-95-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Germ cell mutagenicity (Category 2), H341
Specific target organ toxicity - repeated exposure (Category 2), H373
Acute aquatic toxicity (Category 3), H402
Chronic aquatic toxicity (Category 2), H411

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 Danger

Hazard statement(s)

H227	Combustible liquid.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H314	Causes severe skin burns and eye damage.
H341	Suspected of causing genetic defects.
H373	May cause damage to organs through prolonged or repeated exposure.

H402	Harmful to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

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.
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264	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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Vesicant., Rapidly absorbed through skin.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures

Synonyms : Hydroxybenzene

Formula : C_6H_6O

Molecular weight : 94.11 g/mol

Hazardous components

Component		Classification	Concentration
Phenol			
CAS-No. EC-No. Index-No.	108-95-2 203-632-7 604-001-00-2	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Muta. 2; STOT RE 2; Aquatic Acute 3; Aquatic Chronic 2; H301 + H311 + H331, H314, H318, H341, H373, H402, H411	>= 90 - <= 100 %

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 person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.Continue rinsing eyes during transport to hospital.

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
No data available

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. 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). Keep in suitable, closed containers for disposal.

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.

Handle and store under inert gas. Light sensitive.
Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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

Component	CAS-No.	Value	Control parameters	Basis
Phenol	108-95-2	TWA	5.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation Lung damage Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	5.000000 ppm 19.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		C	15.600000 ppm 60.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption 15 minute ceiling value		
		TWA	5.000000 ppm 19.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m3 is approximate.		
		PEL	5 ppm 19 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Phenol	108-95-2	Phenol	250mg/g Creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	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
Tightly fitting safety goggles. Faceshield (8-inch minimum). 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: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 120 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, 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, 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 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: clear, liquid Colour: colourless, light yellow
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: 38 - 43 °C (100 - 109 °F)
f)	Initial boiling point and boiling range	180 °C (356 °F) at 1,013 hPa (760 mmHg)
g)	Flash point	79 °C (174 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower	Upper explosion limit: 8.6 %(V)

	flammability or explosive limits	Lower explosion limit: 1.8 %(V)
k)	Vapour pressure	No data available
l)	Vapour density	No data available
m)	Relative density	1.060 g/cm3
n)	Water solubility	completely miscible
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	605 °C (1,121 °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
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
Strong bases, Strong oxidizing agents, Strong acids

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
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
Inhalation: No data available

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity

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 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
No data available
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

Additional Information
RTECS: Not available

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence (Phenol)

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
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

Product
This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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: 2821 Class: 6.1 Packing group: II
Proper shipping name: Phenol solutions
Reportable Quantity (RQ): 1111 lbs

Poison Inhalation Hazard: No

IMDG
UN number: 2821 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: PHENOL SOLUTION
Marine pollutant:yes

IATA
UN number: 2821 Class: 6.1 Packing group: II
Proper shipping name: Phenol solution

15. REGULATORY INFORMATION

SARA 302 Components
The following components are subject to reporting levels established by SARA Title III, Section 302:

	CAS-No.	Revision Date
Phenol	108-95-2	2007-07-01

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Phenol	108-95-2	2007-07-01

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Phenol	108-95-2	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Phenol	108-95-2	2007-07-01
Water	7732-18-5	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Phenol	108-95-2	2007-07-01
Water	7732-18-5	

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.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
H227	Combustible liquid.
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled

H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H341	Suspected of causing genetic defects.
H373	May cause damage to organs through prolonged or repeated exposure.
H402	Harmful to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
Muta.	Germ cell mutagenicity
Skin Corr.	Skin corrosion

HMIS Rating

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

NFPA Rating

Health hazard:	3
Fire Hazard:	2
Reactivity Hazard:	0

Further information

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
1-800-521-8956

Version: 3.16 Revision Date: 05/24/2016 Print Date: 03/27/2017

SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 3.10
Revision Date 05/27/2016
Print Date 03/27/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Copper chromite

Product Number : 209317
Brand : Aldrich

CAS-No. : 12053-18-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Oxidizing solids (Category 2), H272
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Acute aquatic toxicity (Category 1), H400
Chronic aquatic toxicity (Category 3), H412

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 Danger

Hazard statement(s)
H272 May intensify fire; oxidizer.
H335 May cause respiratory irritation.
H400 Very toxic to aquatic life.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)
P210 Keep away from heat.
P220 Keep/Store away from clothing/ combustible materials.
P221 Take any precaution to avoid mixing with combustibles.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P271 Use only outdoors or in a well-ventilated area.

P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P304 + P340 + P312	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.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures

Synonyms : Copperchromium oxide

Formula : $Cr_2Cu_2O_5$

Molecular weight : 311.08 g/mol

Hazardous components

Component		Classification	Concentration
Copper chromite			
CAS-No. EC-No.	12053-18-8 235-000-1	Ox. Sol. 2; STOT SE 3; H272, H335	>= 70 - < 90 %
Copper oxide			
CAS-No. EC-No.	1317-38-0 215-269-1	Aquatic Acute 1; Aquatic Chronic 3; H400, H412	>= 20 - < 30 %

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

If swallowed
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
No data available

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 dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. 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-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

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.Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.
Provide appropriate exhaust ventilation at places where dust is formed.Keep away from sources of ignition - No smoking.Keep away from heat and sources of ignition.
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.

Keep in a dry place.
Storage class (TRGS 510): Oxidizing hazardous materials

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

Component	CAS-No.	Value	Control parameters	Basis
Copper chromite	12053-18-8	TWA	0.500000 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Skin irritation Not classifiable as a human carcinogen		

		varies		
		TWA	1.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	1.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	0.5 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Skin irritation Not classifiable as a human carcinogen varies		
		TWA	1 mg/m3	USA. NIOSH Recommended Exposure Limits
Copper oxide	1317-38-0	TWA	0.100000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Also see specific listing for Copper (dusts and mists)		
		TWA	0.100000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Also see specific listing for Copper (dusts and mists)		
		TWA	0.1 mg/m3	USA. NIOSH Recommended Exposure Limits
		Also see specific listing for Copper (dusts and mists)		

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
Safety glasses with side-shields conforming to EN166 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.

Body Protection
Impervious 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 particle respirator type N100 (US) or type P3 (EN 143) 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

a)	Appearance	Form: powder Colour: grey
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	No data available

e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	No data available
g)	Flash point	Not applicable
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	No data available
l)	Vapour density	No data available
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

Bulk density	800 kg/m3

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
Alkali metals, Powdered metals, Reducing agents, Aluminum, Hydrogen sulfide gas

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Copper oxides, Chromium oxides
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
No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity

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 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
No data available
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

Additional Information
RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic 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: 1479 Class: 5.1 Packing group: II
Proper shipping name: Oxidizing solid, n.o.s. (Copper chromite)
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG
UN number: 1479 Class: 5.1 Packing group: II EMS-No: F-A, S-Q
Proper shipping name: OXIDIZING SOLID, N.O.S. (Copper chromite)
Marine pollutant:yes

IATA
UN number: 1479 Class: 5.1 Packing group: II
Proper shipping name: Oxidizing solid, n.o.s. (Copper chromite)

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
Copper chromite	12053-18-8	2007-07-01
Copper oxide	1317-38-0	2007-07-01

SARA 311/312 Hazards
Reactivity Hazard, Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Copper chromite	12053-18-8	2007-07-01
Copper oxide	1317-38-0	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Copper chromite	12053-18-8	2007-07-01
Copper oxide	1317-38-0	2007-07-01

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.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
H272	May intensify fire; oxidizer.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.
Ox. Sol.	Oxidizing solids
STOT SE	Specific target organ toxicity - single exposure

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	2

NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	2
Special hazard.l:	OX

Further information

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
1-800-521-8956

Version: 3.10 Revision Date: 05/27/2016 Print Date: 03/27/2017

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Catechol

SECTION 1 : Identification of the substance/mixture and of the supplier

Product name : **Catechol**

Manufacturer/Supplier Trade name:

Manufacturer/Supplier Article number: **S25680**

Recommended uses of the product and uses restrictions on use:

Manufacturer Details:

AquaPhoenix Scientific
9 Barnhart Drive, Hanover, PA 17331

Supplier Details:

Fisher Science Education
15 Jet View Drive, Rochester, NY 14624

Emergency telephone number:

Fisher Science Education Emergency Telephone No.: 800-535-5053

SECTION 2 : Hazards identification

Classification of the substance or mixture:

Irritant
Skin irritation, category 2
Eye irritation, category 2A
Specific target organ toxicity following single exposure, category 3

Hazards Not Otherwise Classified - Combustible Dust
Skin Irrit. 2
Eye Irrit. 2
STOT SE 3

Signal word :Warning

Hazard statements:
Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation

Precautionary statements:
If medical advice is needed, have product container or label at hand
Keep out of reach of children
Read label before use
Avoid breathing dust/fume/gas/mist/vapours/spray
Use only outdoors or in a well-ventilated area
Wash skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do.
Continue rinsing
Specific treatment (see supplemental first aid instructions on this label)
Remove/Take off immediately all contaminated clothing
IF ON SKIN: Wash with soap and water
If skin irritation occurs: Get medical advice/attention

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Catechol

If eye irritation persists get medical advice/attention
Store in a well ventilated place. Keep container tightly closed
Store locked up
Dispose of contents and container to an approved waste disposal plant

Combustible Dust Hazard: :
May form combustible dust concentrations in air (during processing).

Other Non-GHS Classification:

WHMIS

D1B 

D2B 

NFPA/HMIS

NFPA SCALE (0-4)

Health	3
Flammability	1
Physical Hazard	0
Personal Protection	X

HMIS RATINGS (0-4)

SECTION 3 : Composition/information on ingredients

Ingredients:		
CAS 225937-10-0	Catechol	100 %
		Percentages are by weight

SECTION 4 : First aid measures

Description of first aid measures

After inhalation: Move exposed individual to fresh air. Loosen clothing as necessary and position individual in a comfortable position.Seek medical advice if discomfort or irritation persists.If breathing difficult, give oxygen.

After skin contact: Rinse/flush exposed skin gently using water for 15-20 minutes. Seek medical advice if discomfort or irritation persists.

After eye contact: Protect unexposed eye. Rinse/flush exposed eye(s) gently using water for 15-20 minutes. Remove contact lens(es) if able to do so during rinsing. Seek medical attention if irritation persists or if concerned.

After swallowing: Rinse mouth thoroughly. Do not induce vomiting. Have exposed individual drink sips of water. Seek medical attention if irritation, discomfort or vomiting persists.

Most important symptoms and effects, both acute and delayed:

Irritation, Nausea,Headache, Shortness of breath.;

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Catechol

Indication of any immediate medical attention and special treatment needed:

If seeking medical attention, provide SDS document to physician.

SECTION 5 : Firefighting measures

Extinguishing media

Suitable extinguishing agents: Use water spray . Alcohol-resistant foam . Dry chemical . Carbon dioxide. If in laboratory setting, follow laboratory fire suppression procedures. Use appropriate fire suppression agents for adjacent combustible materials or sources of ignition

For safety reasons unsuitable extinguishing agents:

Special hazards arising from the substance or mixture:

Combustion products may include carbon oxides or other toxic vapors.Avoid generating dust; fine dust dispersed in air in sufficient concentrations, and in the presence of an ignition source is a potential dust explosion hazard.

Advice for firefighters:

Protective equipment: Wear self contained breathing apparatus for fire fighting if necessary.Use NIOSH-approved respiratory protection/breathing apparatus.

Additional information (precautions): Move product containers away from fire or keep cool with water spray as a protective measure, where feasible.Use spark-proof tools and explosion-proof equipment.

SECTION 6 : Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Use personal protective equipment.Ensure adequate ventilation.Keep away from ignition sources. Transfer to a disposal or recovery container. Avoid dust formation. Use spark-proof tools and explosion-proof equipment.Use respiratory protective device against the effects of fumes/dust/aerosol.

Environmental precautions:

Do not let product enter drains.Collect contaminated soil for characterization per Section 13

Methods and material for containment and cleaning up:

If in a laboratory setting, follow Chemical Hygiene Plan procedures.Place into properly labeled containers for recovery or disposal. Avoid dispersal of dust in the air (i.e., clearing dust surfaces with compressed air). Collect solids in powder form using vacuum with (HEPA filter)

Reference to other sections:

SECTION 7 : Handling and storage

Precautions for safe handling:

Avoid contact with skin and eyes. Use only in well ventilated areas.Avoid generation of dust or fine particulate.Avoid contact with eyes, skin, and clothing. Wash hands after handling. Minimize dust generation and accumulation. Dry powders can build static electricity charges when subjected to the friction of transfer and mixing operations. Follow good hygiene procedures when handling chemical materials. Do not eat, drink, smoke, or use personal products when handling chemical substances.

Conditions for safe storage, including any incompatibilities:

Store in cool place. Store with like hazards. Provide ventilation for containers. Store away from foodstuffs. Store away from oxidizing agents.Store in cool, dry conditions in well sealed containers.

SECTION 8 : Exposure controls/personal protection

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Catechol

Control Parameters: , , OSHA PEL TWA (Total Dust) 15 mg/m3 (50 mppcf*)
, , ACGIH TLV TWA (inhalable particles) 10 mg/m3

Appropriate Engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.Emergency eye wash fountains and safety showers should be available in the immediate vicinity of use/handling.Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapor or dusts (total/respirable) below the applicable workplace exposure limits (Occupational Exposure Limits-OELs) indicated above.Use under a fume hood. It is recommended that all dust control equipment such as local exhaust ventilation and material transport systems involved in handling of this product contain explosion relief vents or an explosion suppression system or an oxygen deficient environment.Ensure that dust-handling systems (such as exhaust ducts, dust collectors, vessels, and processing equipment) are designed in a manner to prevent the escape of dust into the work area (i.e., there is no leakage from the equipment).

Respiratory protection: Not required under normal conditions of use. Use suitable respiratory protective device when high concentrations are present. Use suitable respiratory protective device when aerosol or mist is formed. For spills, respiratory protection may be advisable.

Protection of skin: The glove material has to be impermeable and resistant to the product/ the substance/ the preparation being used/handled.Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation.

Eye protection: Safety glasses with side shields or goggles.

General hygienic measures: The usual precautionary measures are to be adhered to when handling chemicals. Keep away from food, beverages and feed sources. Immediately remove all soiled and contaminated clothing. Wash hands before breaks and at the end of work. Do not inhale gases/fumes/dust/mist/vapor/aerosols. Avoid contact with the eyes and skin.

SECTION 9 : Physical and chemical properties

Appearance (physical state,color):	Almost white to brown solid.	**Explosion limit lower**: **Explosion limit upper**:	Not Determined Not Determined
Odor:	Phenol - like	**Vapor pressure**:	0.01 mm Hg @ 25 C
Odor threshold:	Not Determined	**Vapor density**:	3.8
pH-value:	Not Determined	**Relative density**:	1.344
Melting/Freezing point:	103 - 106 C	**Solubilities**:	Material is water soluble.
Boiling point/Boiling range:	245 C	**Partition coefficient (n-octanol/water)**:	Not Determined
Flash point (closed cup):	127 C	**Auto/Self-ignition temperature**:	Not Determined

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Evaporation rate:	Not Determined	**Decomposition temperature**:	Not Determined
Flammability (solid,gaseous):	Not Determined	**Viscosity**:	a. Kinematic:Not Determined b. Dynamic: Not Determined
Density: Not Determined **Catechol:**Molecular Weight: 110.11			

SECTION 10 : Stability and reactivity

Reactivity:
Chemical stability: Substance undergoes color change upon exposure to light and air. Substance sublimes.
Possible hazardous reactions: None under normal processing.
Conditions to avoid: Store away from oxidizing agents, strong acids or bases.Light, dust generation, prolonged exposure to air, excess heat.
Incompatible materials: Strong oxidizers, aluminum.
Hazardous decomposition products: Carbon oxides (CO, CO2).

SECTION 11 : Toxicological information

Acute Toxicity:		
Oral:	26 0 mg/kg	LD50 orl - rat
Chronic Toxicity: No additional information.		
Corrosion Irritation: No additional information.		
Sensitization:		No additional information.
Single Target Organ (STOT):		No additional information.
Numerical Measures:		No additional information.
Carcinogenicity:		Catechol: ACGIH: A3 – Confirmed animal carcinogen with unknown relevance to humans, IARC: Group 2
Mutagenicity:		No additional information.
Reproductive Toxicity:		No additional information.

SECTION 12 : Ecological information

Ecotoxicity Persistence and degradability: Readily degradable in the environment.
Bioaccumulative potential:
Mobility in soil:
Other adverse effects:

SECTION 13 : Disposal considerations

Waste disposal recommendations:
It is the responsibility of the waste generator to properly characterize all waste materials according to

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Catechol

applicable regulatory entities (US 40CFR262.11). Consult federal state/ provincial and local regulations regarding the proper disposal of waste material that may incorporate some amount of this product.

SECTION 14 : Transport information

UN-Number

2811

UN proper shipping name

Toxic solids , Organic , N.O.S .

Transport hazard class(es)

Class:
6.1 Toxic substances

Packing group:III
Environmental hazard:
Transport in bulk:
Special precautions for user:

SECTION 15 : Regulatory information

United States (USA)

SARA Section 311/312 (Specific toxic chemical listings):

Acute

SARA Section 313 (Specific toxic chemical listings):

225937-10-0 Catechol

RCRA (hazardous waste code):

None of the ingredients is listed

TSCA (Toxic Substances Control Act):

All ingredients are listed.

CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act):

225937-10-0 Catechol 100 lb

Proposition 65 (California):

Chemicals known to cause cancer:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for females:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for males:

None of the ingredients is listed

Chemicals known to cause developmental toxicity:

None of the ingredients is listed

Canada

Canadian Domestic Substances List (DSL):

All ingredients are listed.

Canadian NPRI Ingredient Disclosure list (limit 0.1%):

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Catechol

None of the ingredients is listed

Canadian NPRI Ingredient Disclosure list (limit 1%):

None of the ingredients is listed

SECTION 16 : Other information

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations.Note:. The responsibility to provide a safe workplace remains with the user.The user should consider the health hazards and safety information contained herein as a guide and should take those precautions required in an individual operation to instruct employees and develop work practice procedures for a safe work environment.The information contained herein is, to the best of our knowledge and belief, accurate.However, since the conditions of handling and use are beyond our control, we make no guarantee of results, and assume no liability for damages incurred by the use of this material.It is the responsibility of the user to comply with all applicable laws and regulations applicable to this material.

GHS Full Text Phrases:

Abbreviations and acronyms:
IMDG: International Maritime Code for Dangerous Goods
PNEC: Predicted No-Effect Concentration (REACH)
CFR: Code of Federal Regulations (USA)
SARA: Superfund Amendments and Reauthorization Act (USA)
RCRA: Resource Conservation and Recovery Act (USA)
TSCA: Toxic Substances Control Act (USA)
NPRI: National Pollutant Release Inventory (Canada)
DOT: US Department of Transportation
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
ACGIH: American Conference of Governmental Industrial Hygienists
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
DNEL: Derived No-Effect Level (REACH)

Effective date : 01.20.2015
Last updated : 03.19.2015

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Benzoic Acid

SECTION 1 : Identification of the substance/mixture and of the supplier

Product name : **Benzoic Acid**

Manufacturer/Supplier Trade name:

Manufacturer/Supplier Article number: **S25195**

Recommended uses of the product and uses restrictions on use:

Manufacturer Details:

AquaPhoenix Scientific
9 Barnhart Drive, Hanover, PA 17331

Supplier Details:

Fisher Science Education
15 Jet View Drive, Rochester, NY 14624

Emergency telephone number:

Fisher Science Education Emergency Telephone No.: 800-535-5053

SECTION 2 : Hazards identification

Classification of the substance or mixture:

Corrosive
Serious eye damage, category 1

Health hazard
Specific target organ toxicity following repeated exposure, category 1

Irritant
Skin irritation, category 2

skin corr./irrit. 2
Serious eye dam. 1
STOT RE 1
Hazards Not Otherwise Classified - Combustible Dust

Signal word :Danger

Hazard statements:
Causes skin irritation
Causes serious eye damage
Causes damage to organs through prolonged or repeated exposure
Precautionary statements:
If medical advice is needed, have product container or label at hand
Keep out of reach of children
Read label before use
Wear protective gloves/protective clothing/eye protection/face protection
Do not breathe dust/fume/gas/mist/vapours/spray
Wash ... thoroughly after handling

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Benzoic Acid

Do not eat, drink or smoke when using this product
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing
IF ON SKIN: Wash with soap and water
Take off contaminated clothing and wash before reuse
If skin irritation occurs: Get medical advice/attention
Immediately call a POISON CENTER or doctor/physician
Specific treatment (see ... on this label)
Dispose of contents/container to ...

Combustible Dust Hazard: :
May form combustible dust concentrations in air (during processing).

Other Non-GHS Classification:

WHMIS

D2B 

E 

NFPA/HMIS

NFPA SCALE (0-4)

Health	2
Flammability	0
Physical Hazard	0
Personal Protection	X

HMIS RATINGS (0-4)

SECTION 3 : Composition/information on ingredients

Ingredients:		
CAS 65-85-0	Benzoic Acid	>99 %
		Percentages are by weight

SECTION 4 : First aid measures

Description of first aid measures

After inhalation: Move exposed individual to fresh air. Loosen clothing as necessary and position individual in a comfortable position.Seek medical advice if discomfort or irritation persists.If breathing difficult, give oxygen.

After skin contact: Wash affected area with soap and water. Rinse/flush exposed skin gently using water for 15-20 minutes. Seek medical advice if discomfort or irritation persists.

After eye contact: Protect unexposed eye. Remove contact lens(es) if able to do so during rinsing. Rinse or flush eye gently with water for at least 30 minutes, lifting upper and lower lids.Seek immediate medical attention (ophthalmologist)

After swallowing: Rinse mouth thoroughly. Do not induce vomiting. Have exposed individual drink sips of

water. Seek medical attention if irritation, discomfort or vomiting persists.

Most important symptoms and effects, both acute and delayed:

Irritation, Nausea,Headache, Shortness of breath.Diarrhea. Vomiting. Irritation/burns, all routes of exposure.May cause permanent eye injury.;Prolonged or repeated skin contact may cause dermatitis.

Indication of any immediate medical attention and special treatment needed:

If seeking medical attention, provide SDS document to physician.

SECTION 5 : Firefighting measures

Extinguishing media

Suitable extinguishing agents: Carbon dioxide. Dry chemical powder. Alcohol foam. Polymer foam. If in laboratory setting, follow laboratory fire suppression procedures. Use appropriate fire suppression agents for adjacent combustible materials or sources of ignition

For safety reasons unsuitable extinguishing agents: Water spray may be ineffective.

Special hazards arising from the substance or mixture:

Combustion products may include carbon oxides or other toxic vapors.Thermal decomposition can lead to release of irritating gases and vapors.Avoid generating dust; fine dust dispersed in air in sufficient concentrations, and in the presence of an ignition source is a potential dust explosion hazard.

Advice for firefighters:

Protective equipment: Use NIOSH-approved respiratory protection/breathing apparatus.

Additional information (precautions): Move product containers away from fire or keep cool with water spray as a protective measure, where feasible.Use spark-proof tools and explosion-proof equipment.

SECTION 6 : Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Wear protective equipment. Transfer to a disposal or recovery container.Use spark-proof tools and explosion-proof equipment.Use respiratory protective device against the effects of fumes/dust/aerosol. Keep unprotected persons away. Ensure adequate ventilation.Keep away from ignition sources. Protect from heat.Stop the spill, if possible. Contain spilled material by diking or using inert absorbent.

Environmental precautions:

Prevent from reaching drains, sewer or waterway. Collect contaminated soil for characterization per Section 13

Methods and material for containment and cleaning up:

If in a laboratory setting, follow Chemical Hygiene Plan procedures.Place into properly labeled containers for recovery or disposal. If necessary, use trained response staff/contractor.Dust deposits should not be allowed to accumulate on surfaces, as these may form an explosive mixture if they are released into the atmosphere in sufficient concentration. Avoid dispersal of dust in the air (i.e., clearing dust surfaces with compressed air). Collect solids in powder form using vacuum with (HEPA filter)

Reference to other sections:

SECTION 7 : Handling and storage

Precautions for safe handling:

Minimize dust generation and accumulation. Wash hands after handling. Avoid dispersal of dust in the air (i.e., clearing dust surfaces with compressed air). Routine housekeeping should be instituted to ensure that dusts do not accumulate on surfaces. Dry powders can build static electricity charges when subjected to the friction of transfer and mixing operations. Follow good hygiene procedures when handling chemical materials. Do not eat, drink, smoke, or use personal products when handling chemical substances. If in a laboratory setting, follow Chemical Hygiene Plan.Use only in well ventilated areas.Avoid generation of dust or fine particulate.Avoid

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Benzoic Acid

contact with eyes, skin, and clothing.

Conditions for safe storage, including any incompatibilities:

Store in a cool location. Provide ventilation for containers. Avoid storage near extreme heat, ignition sources or open flame. Store away from foodstuffs. Store away from oxidizing agents.Store in cool, dry conditions in well sealed containers. Keep container tightly sealed.Store with like hazards

SECTION 8 : Exposure controls/personal protection

Control Parameters: , , OSHA PEL TWA (Total Dust) 15 mg/m3 (50 mppcf*)
, , ACGIH TLV TWA (inhalable particles) 10 mg/m3

Appropriate Engineering controls: Emergency eye wash fountains and safety showers should be available in the immediate vicinity of use/handling.Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapor or dusts (total/respirable) below the applicable workplace exposure limits (Occupational Exposure Limits-OELs) indicated above.Use under a fume hood. It is recommended that all dust control equipment such as local exhaust ventilation and material transport systems involved in handling of this product contain explosion relief vents or an explosion suppression system or an oxygen deficient environment.Ensure that dust-handling systems (such as exhaust ducts, dust collectors, vessels, and processing equipment) are designed in a manner to prevent the escape of dust into the work area (i.e., there is no leakage from the equipment).

Respiratory protection: Use suitable respiratory protective device when high concentrations are present. Use suitable respiratory protective device when aerosol or mist is formed. For spills, respiratory protection may be advisable. Not required under normal conditions of use with adequate ventilation.

Protection of skin: The glove material has to be impermeable and resistant to the product/ the substance/ the preparation being used/handled.Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation.

Eye protection: Safety glasses with side shields or goggles.

General hygienic measures: The usual precautionary measures are to be adhered to when handling chemicals. Keep away from food, beverages and feed sources. Immediately remove all soiled and contaminated clothing. Wash hands before breaks and at the end of work. Do not inhale gases/fumes/dust/mist/vapor/aerosols. Avoid contact with the eyes and skin.

SECTION 9 : Physical and chemical properties

Appearance (physical state,color):	Crystalline powder	**Explosion limit lower**: **Explosion limit upper**:	Not Determined Not Determined
Odor:	Pleasant odor	**Vapor pressure**:	0.0012 mm Hg @ 25C
Odor threshold:	Not Determined	**Vapor density**:	4.21 (air=1)
pH-value:	2.8 (satd soln)	**Relative density**:	Not Determined

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Benzoic Acid

Melting/Freezing point:	122.4 deg C	**Solubilities**:	3.4 g/l @ 25C
Boiling point/Boiling range:	249.2C @ 760 mmHg	**Partition coefficient (n-octanol/water)**:	Not Determined
Flash point (closed cup):	121C	**Auto/Self-ignition temperature**:	570C
Evaporation rate:	Negligible	**Decomposition temperature**:	Not Determined
Flammability (solid,gaseous):	Not Determined	**Viscosity**:	a. Kinematic:Not Determined b. Dynamic: Not Determined
Density: Not Determined			

SECTION 10 : Stability and reactivity

Reactivity:
Chemical stability: No decomposition if used and stored according to specifications.
Possible hazardous reactions:
Conditions to avoid: Store away from oxidizing agents, strong acids or bases.Dust generation. Excess heat
Incompatible materials: Strong bases.Strong oxidizing and reducing agents
Hazardous decomposition products: Carbon oxides (CO, CO2).Phenol, benzene.

SECTION 11 : Toxicological information

Acute Toxicity:		
Oral:	1700 mg/kg	Oral LD50 Rat
Inhalation:	> 12.2 mg/l	LC50 Inhalation - rat - 4 h
Dermal:	> 10,000 mg/kg	LD50 Dermal - rabbit
Chronic Toxicity: No additional information.		
Corrosion Irritation:		
Dermal:	Section 2	Classified as Skin Irritant
Ocular:	Section 2	Classified as Serious Eye Damage
Sensitization:		No additional information.
Single Target Organ (STOT):		Classified as STOT RE 1
Numerical Measures:		No additional information.
Carcinogenicity:		No additional information.
Mutagenicity:		No additional information.
Reproductive Toxicity:		No additional information.

SECTION 12 : Ecological information

Ecotoxicity

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Benzoic Acid

Water Flea: 48 Hr EC50 Daphnia magna: 860 mg/L [Static]

Fish:: Mosquito Fish: LC50 = 180 mg/L; 96 Hr;

UnspecifiedBacteria: : Phytobacterium phosphoreum: EC50 = 16.9 mg/L; 96 Hr; Microtox test @ 15°C

Persistence and degradability: Readily degradable in the environment. If released on land, benzoic acid should leach into the ground due to its low soil adsorption and biodegrade (half-life <1 wk). If released in water, benzoic acid should also readily biodegrade (half-life 0.2-3.6 days).
Bioaccumulative potential:
Mobility in soil: Adsorption to sediment and volatilization should not be significant.
Other adverse effects:

SECTION 13 : Disposal considerations

Waste disposal recommendations:

Product/containers must not be disposed together with household garbage. Do not allow product to reach sewage system or open water.It is the responsibility of the waste generator to properly characterize all waste materials according to applicable regulatory entities (US 40CFR262.11). Consult federal state/ provincial and local regulations regarding the proper disposal of waste material that may incorporate some amount of this product.

SECTION 14 : Transport information

UN-Number

Not Regulated

UN proper shipping name

Not Regulated

Transport hazard class(es)
Packing group:Not Regulated
Environmental hazard:
Transport in bulk:
Special precautions for user:

SECTION 15 : Regulatory information

United States (USA)

SARA Section 311/312 (Specific toxic chemical listings):

Acute, Chronic

SARA Section 313 (Specific toxic chemical listings):

None of the ingredients is listed

RCRA (hazardous waste code):

None of the ingredients is listed

TSCA (Toxic Substances Control Act):

All ingredients are listed.

CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act):

65-85-0 Benzoic acid 5000 lb (2270 kg)

Proposition 65 (California):

Chemicals known to cause cancer:

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Benzoic Acid

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for females:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for males:

None of the ingredients is listed

Chemicals known to cause developmental toxicity:

None of the ingredients is listed

Canada

Canadian Domestic Substances List (DSL):

All ingredients are listed.

Canadian NPRI Ingredient Disclosure list (limit 0.1%):

None of the ingredients is listed

Canadian NPRI Ingredient Disclosure list (limit 1%):

None of the ingredients is listed

SECTION 16 : Other information

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations.Note:. The responsibility to provide a safe workplace remains with the user.The user should consider the health hazards and safety information contained herein as a guide and should take those precautions required in an individual operation to instruct employees and develop work practice procedures for a safe work environment.The information contained herein is, to the best of our knowledge and belief, accurate.However, since the conditions of handling and use are beyond our control, we make no guarantee of results, and assume no liability for damages incurred by the use of this material.It is the responsibility of the user to comply with all applicable laws and regulations applicable to this material.

GHS Full Text Phrases:

Abbreviations and acronyms:
IMDG: International Maritime Code for Dangerous Goods
PNEC: Predicted No-Effect Concentration (REACH)
CFR: Code of Federal Regulations (USA)
SARA: Superfund Amendments and Reauthorization Act (USA)
RCRA: Resource Conservation and Recovery Act (USA)
TSCA: Toxic Substances Control Act (USA)
NPRI: National Pollutant Release Inventory (Canada)
DOT: US Department of Transportation
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
ACGIH: American Conference of Governmental Industrial Hygienists
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
DNEL: Derived No-Effect Level (REACH)

Effective date : 12.29.2014
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SIGMA-ALDRICH

sigma-aldrich.com

SAFETY DATA SHEET

Version 5.3
Revision Date 02/26/2015
Print Date 03/27/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Benzaldehyde

Product Number : B6259
Brand : Sigma
Index-No. : 605-012-00-5

CAS-No. : 100-52-7

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 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Respiratory sensitisation (Category 1), H334
Skin sensitisation (Category 1), H317
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

Pictogram

Signal word Danger

Hazard statement(s)

H227	Combustible liquid.
H302 + H312	Harmful if swallowed or in contact with skin
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H401	Toxic to aquatic life.

Precautionary statement(s)	
P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P341	IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/ physician.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Artificial essential oil of almond
Formula	:	C_7H_6O
Molecular weight	:	106.12 g/mol
CAS-No.	:	100-52-7
EC-No.	:	202-860-4
Index-No.	:	605-012-00-5

Hazardous components

Component	Classification	Concentration
Benzaldehyde		
	Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Resp. Sens. 1; Skin Sens. 1; Aquatic Acute 2; H227, H302 + H312, H315, H317, H334, H401	<= 100 %

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 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
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

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Under fire conditions, material may decompose to form flammable and/or explosive mixtures in air.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 13). Keep in suitable, closed containers for disposal.

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 under nitrogen. 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.

Air, light, and moisture 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

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Benzaldehyde	100-52-7	TWA	2.000000 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
	Remarks	Dermal Sensitization Notation		
		STEL	4.000000 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
		Dermal Sensitization Notation		

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 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: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Chloroprene
Minimum layer thickness: 0.6 mm
Break through time: 35 min
Material tested:Camapren® (KCL 722 / Aldrich Z677493, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, 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, 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 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	5.9 at 20 °C (68 °F)
e)	Melting point/freezing point	-26 °C (-15 °F)
f)	Initial boiling point and boiling range	177 - 179 °C (351 - 354 °F)
g)	Flash point	64 °C (147 °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: 8.5 %(V) Lower explosion limit: 1.4 %(V)
k)	Vapour pressure	5 hPa (4 mmHg) at 45 °C (113 °F)
l)	Vapour density	3.66 - (Air = 1.0)
m)	Relative density	1.050 g/cm3
n)	Water solubility	slightly soluble
o)	Partition coefficient: n-octanol/water	log Pow: 1.5
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	3.66 - (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
Air Exposure to moisture Light. Heat
Heat, flames and sparks.

10.5 Incompatible materials
Strong oxidizing agents, Strong reducing agents, Strong bases, Alkali metals, Aluminium, Iron, phenols, Oxygen

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 - 1,300 mg/kg
Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Coma.

Inhalation: No data available

LD50 Dermal - Rabbit - 1,250 mg/kg

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - 24 h

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Mild eye irritation

Respiratory or skin sensitisation
Germ cell mutagenicity
Laboratory experiments have shown mutagenic effects.

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen 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

Aspiration hazard
No data available

Additional Information
RTECS: CU4375000

Central nervous system depression, Prolonged or repeated exposure to skin causes defatting and dermatitis.

Liver - Irregularities - Based on Human Evidence
Liver - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	LC50 - Lepomis macrochirus - 1.07 mg/l - 96 h
	mortality LOEC - Pimephales promelas (fathead minnow) - 0.45 mg/l - 7 d
	mortality NOEC - Pimephales promelas (fathead minnow) - 0.22 mg/l - 7 d
	LC50 - Leuciscus idus (Golden orfe) - 62 mg/l - 48 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 50 mg/l - 24 h

12.2 Persistence and degradability

Biodegradability: Biotic/Aerobic - Exposure time 28 d
Result: 95 % - 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.
Toxic to aquatic life.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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: 1990 Class: 9 Packing group: III
Proper shipping name: Benzaldehyde
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 1990 Class: 9 Packing group: III EMS-No: F-A, S-A
Proper shipping name: BENZALDEHYDE

IATA

UN number: 1990 Class: 9 Packing group: III
Proper shipping name: Benzaldehyde

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, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Benzaldehyde	100-52-7	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Benzaldehyde	100-52-7	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Benzaldehyde	100-52-7	2007-03-01

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.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Flam. Liq.	Flammable liquids
H227	Combustible liquid.
H302	Harmful if swallowed.
H302 + H312	Harmful if swallowed or in contact with skin
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

Further information

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
1-800-521-8956

Version: 5.3 Revision Date: 02/26/2015 Print Date: 03/27/2017

Appendix 4

Equipment Design Calculations

Appendix 4.1: Compressor, Pump, and Turbine Head and Power Requirements

Head was calculated from pressure changes across the process unit and the density ρ of the fluid passing through. A pressure change of 25 psi was assumed for the normal movement of fluid through the reflux and shutdown pumps in each distillation column. Pump and motor efficiencies for these six pumps were determined based on the operating volumetric flowrate Q in gallons per minute. The electricity consumption in kWh was then determined from the brake horsepower. Net power requirements and head for the feed and recycle pumps, and air compressor, were taken directly from ASPEN in units of horsepower and feet. Net electricity produced by the two turbines was also taken directly from ASPEN in units of kilowatts.

Sample Calculation using P-302

$$Head\ (H) = \frac{2.31 * Pressure\ Change}{Fluid\ Specific\ Gravity} = \frac{(25\ psi) * 2.31}{\left(6.82\frac{lb}{gal} \Big/ 8.33\frac{lb}{gal}\right)} = 70.6\ ft \quad \text{(A1)}$$

$$Pump\ Efficiency\ (\eta_P) = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2 \quad \text{(A2)}$$

$$= -0.316 + 0.24015(\ln 483\ gpm) - 0.01199(\ln 483\ gpm)^2 = 0.710$$

$$Brake\ Horsepower\ (P_B) = \frac{QH\rho}{33{,}000\eta_P} = \frac{483\ gpm * 70.6\ ft * 6.28\frac{lb}{gal}}{33{,}000 * 0.71} = 9.92\ hp \quad \text{(A3)}$$

$$Electric\ Motor\ Efficiency\ (\eta_M) = 0.80 + 0.0319(\ln P_B) - 0.00182(\ln P_B)^2$$

$$= 0.80 + 0.319(\ln 9.92\ hp) - 0.00182(\ln 9.92\ hp)^2 = 0.864 \quad \text{(A4)}$$

$$Electric\ Consumption\ (P_C) = \frac{P_B}{\eta_M} * \frac{0.7457\ kW}{hp} * 1\ hr = \frac{9.92\ hp}{0.864} * \frac{0.7457\ kW}{hp} * 1\ hr$$

$$= 8.57\ kWh \quad \text{(A5)}$$

Appendix 4.2.1 Process Heat Exchanger Sizing and Utilities

Surface areas for all heat exchangers in the process, excluding the main counter-current effluent heat exchanger E-201, were approximated using heat duties $\dot{Q}$, appropriate LMTD temperature approaches, and heat transfer coefficients U estimated from *Seider et. al, 2017*[A4.1] . All exchanger heat duties, except for heated storage pump-arounds E-505, E-506, E-507, were taken from ASPEN. See Appendix 4.6, pg. 221 for heat duty calculations on the storage tanks. Temperature changes for cooling water streams were taken to be from 86 °F to 104 °F. We assumed that all of the energy taken from steam, or given to boiler feed water, comes from the respective processes of condensation and vaporization. Low pressure steam temperature for condensation and boiler feed water temperature for steam formation were both taken to be constant at 250 °F, the saturation temperature of 15 psig steam. High pressure steam temperature for condensation was taken to be constant at 470 °F, the saturation temperature of 500 psig steam. Utility flows were determined based on the exchanger heat duty and either the heat of vaporization of the utility stream, or the constant pressure heat capacity c_p and allowed temperature change of the utility stream.

Sample Calculation using E-302

$$LMTD = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} = \frac{(285\ °\text{F} - 104\ °\text{F}) - (110\ °\text{F} - 86\ °\text{F})}{\ln\left(\frac{(285\ °\text{F} - 104\ °\text{F})}{(110\ °\text{F} - 86\ °\text{F})}\right)} = 78\ °\text{F} \qquad \text{(A6)}$$

[A4.1] Seider, W.D., J.D. Seader, D.R. Lewin, and S. Widago, "Product and Process Design Principles", John Wiley & Sons Inc., New Jersey, 2017, pg.376.

$$Surface\ Area\ (A) = \frac{\dot{Q}}{U * LMTD} = \frac{24{,}827{,}573\,\frac{BTU}{hr}}{60\,\frac{BTU}{°\mathrm{F} - ft^2 - hr} * 78\ °\mathrm{F}} = 5325\ ft^2 \qquad \text{(A7)}$$

$$Utility\ Mass\ Flow\ (m) = \frac{\dot{Q}}{c_p * \Delta T} = \frac{24{,}827{,}573\,\frac{BTU}{hr}}{1\,\frac{BTU}{lb - °\mathrm{F}} * 18\ °\mathrm{F}} \qquad \text{(A8)}$$

$$= 1{,}379{,}310\,\frac{lb}{hr}\,cooling\ water$$

Appendix 4.2.2 Tubular Exchanger Manufacturers Association (TEMA) Specification Sheet

Aspen Exchanger Design and Rating Shell & Tube V9

File: E-201_1.edr Printed: 4/6/2017 at 11:21:32 AM

TEMA Sheet

Heat Exchanger Specification Sheet

1	Company:											
2	Location:											
3	Service of Unit:		Our Reference:									
4	Item No.:		Your Reference:									
5	Date:	Rev No.:	Job No.:									
6	Size: 40 - 360	in	Type: DEU	Horizontal			Connected in: 1 parallel	1 series				
7	Surf/unit(eff.)	8401.5	ft²	Shells/unit 1			Surf/shell(eff.)	8401.5	ft²			
8	**PERFORMANCE OF ONE UNIT**											
9	Fluid allocation			Shell Side			Tube Side					
10	Fluid name			5			8					
11	Fluid quantity, Total		lb/h	453112			509683					
12	Vapor (In/Out)		lb/h	0	0		509683	190457				
13	Liquid		lb/h	453112	453112		0	319226				
14	Noncondensable		lb/h	0	0		0	0				
15												
16	Temperature (In/Out)		°F	165.03	491.61		662	441.48				
17	Dew / Bubble point		°F	540.13	539.78		515.78	-41.06				
18	Density Vapor/Liquid		lb/ft³	/ 51.285	/ 30.569		3.987 /	4.02 / 40.451				
19	Viscosity		cp	/ 0.3411	/ 0.0824		0.0191 /	0.0181 / 0.0877				
20	Molecular wt, Vap						68.86	56.33				
21	Molecular wt, NC											
22	Specific heat		BTU/(lb-F)	/ 0.4129	/ 1.7779		0.5126 /	0.4275 / 0.6231				
23	Thermal conductivity		BTU/(ft-h-F)	/ 0.074	/ 0.042		0.024 /	0.018 / 0.05				
24	Latent heat		BTU/lb				94.6	101.2				
25	Pressure (abs)		psi	652.86	651.13		594.85	590.37				
26	Velocity (Mean/Max)		ft/s	2.14 / 3.73			14.61 / 24.19					
27	Pressure drop, allow./calc.		psi	10	1.73		10	4.48				
28	Fouling resistance (min)		ft²-h-F/BTU	0.002			0.002	0.0024 Ao based				
29	Heat exchanged	88350260	BTU/h				MTD (corrected)	122.76	°F			
30	Transfer rate, Service	85.67		Dirty	84.92		Clean	135.94	BTU/(h-ft²-F)			
31	**CONSTRUCTION OF ONE SHELL**								**Sketch**			
32				Shell Side			Tube Side					
33	Design/Vacuum/test pressure		psi	725.19 / /			667.17 / /					
34	Design temperature		°F	725			725					
35	Number passes per shell			1			2					
36	Corrosion allowance		in	0			0					
37	Connections	In	in	1 10.02 / -			1 17.25 / -					
38	Size/Rating	Out		1 13.25 / -			1 12 / -					
39	ID	Intermediate		/ -			/ -					
40	Tube No. 700	Us OD 0.75	TksAverage 0.065		in Length 360			in Pitch 0.9375	in			
41	Tube type Plain			#/in	Material SS 316			Tube pattern 30				
42	Shell SS 316		ID 40	OD 42.2047	in		Shell cover SS 316					
43	Channel or bonnet	SS 316					Channel cover SS 316					
44	Tubesheet-stationary	SS 316	-				Tubesheet-floating -					
45	Floating head cover	-					Impingement protection None					
46	Baffle-cross SS 316		Type Single segmental		Cut(%d) 28.92		Horiz.Spacing: c/c 25		in			
47	Baffle-long -		Seal Type				Inlet 0		in			
48	Supports-tube	U-bend	0				Type					
49	Bypass seal			Tube-tubesheet joint			Expanded only (2 grooves)(App.A 'I')					
50	Expansion joint	-		Type None								
51	RhoV2-Inlet nozzle 1030		Bundle entrance 396				Bundle exit 41		lb/(ft-s²)			
52	Gaskets - Shell side	Flat Metal Jacket Fibe		Tube side	Flat Metal Jacket Fibe							
53	Floating head	-										
54	Code requirements	ASME Code Sec VIII Div 1			TEMA class R - refinery service							
55	Weight/Shell	50255.7	Filled with water 65737.6		Bundle 24055.6		lb					
56	Remarks											
57												
58												

Appendix 4.3 Reactor Pressure and Sizing

The procedure for determining reactor pressure, sizing, and number of stages is described in detail in Section 13.3, pg. 57 and Section 15.1.3, pg. 76. The procedure is briefly summarized here. All catalyst properties were assumed to be that of bulk alumina with bulk density ρ_{bulk}, bed porosity ε, and particle diameter d_p. ASPEN was used to determine the overall adiabatic temperature rise of 216 °F, which led us to set a reasonable temperature rise of 54 °F across each of 4 reactor stages, with 3 intercoolers used to maintain the temperature range. An L/D ratio of 4 for a vertical reactor was set to conserve space. An LHSV of 100 $\frac{mL\ benzene}{hr*g_{catalyst}}$ =1.60 $\frac{ft^3\ benzene}{hr*lb_{catalyst}}$was taken from the patent. Total mass of catalyst was calculated from LHSV and volumetric flowrate $\dot{V}$. Reactor volume was determined from catalyst volume and a 10% safety factor. This total volume was used to find reactor residence times, diameter, and consequently the height of the overall reactor and of each reactor section. The Ergun equation with fluid viscosity μ and fluid density ρ was used to find a reasonable pressure drop set across each stage, as well as an overall pressure drop.

Sample Calculations using R-201A/B

$$\frac{L}{D} = 4 \tag{A9}$$

$$m_{cat_{tot}} = \frac{\dot{V}}{LHSV} = \frac{38.58\frac{ft^3}{s}}{100\frac{ml}{hr - g_{cat}}} * \frac{3600\ s}{hr} * \frac{28317\ ml}{ft^3} * \frac{2.205\ lb}{kg} * \frac{1\ kg}{1000\ g_{cat}}$$

$$= 86{,}707\ lb \tag{A10}$$

$$m_{cat_{section}} = \frac{m_{cat_{tot}}}{4} = \frac{86{,}707\ lb}{4} = 21{,}677\ lb \tag{A11}$$

$$V_{tot} = \frac{m_{cat_{tot}} * Safety\ Factor}{\rho_{bulk}} = \frac{86{,}707\ lb * 1.1}{40.02\frac{lb}{ft^3}} = 2384\ ft^3 \quad \text{(A12)}$$

$$Total\ Residence\ Time\ (\tau_{tot}) = \frac{V_{tot}}{\dot{V}} = \frac{2384\ ft^3}{38.58\frac{ft^3}{s}} * \frac{min}{60\ sec} = 1.03\ min \quad \text{(A13)}$$

$$\tau_{section} = \frac{\tau_{tot}}{4} = \frac{1.03\ min}{4} * \frac{60\ sec}{min} = 15.4\ sec \quad \text{(A14)}$$

$$D = \left(\frac{V_{tot}}{\pi}\right)^{1/3} = \left(\frac{2384\ ft^3}{\pi}\right)^{1/3} = 9.12\ ft \quad \text{(A15)}$$

$$L_{tot} = 4 * D = 4 * (9.12ft) = 36.5\ ft \quad \text{(A16)}$$

$$L_{section} = \frac{L_{tot}}{4} = 9.12\ ft \quad \text{(A17)}$$

$$Cross\ Sectional\ Area\ (A) = \frac{\pi D^2}{4} = \frac{\pi * (9.12\ ft)^2}{4} = 65.3\ ft^2 \quad \text{(A18)}$$

$$Superficial\ Fluid\ Velocity\ (u_0) = \frac{\dot{V}}{A} = \frac{38.58\frac{ft^3}{s}}{65.3\ ft^2} = 0.591\frac{ft}{s} \quad \text{(A19)}$$

Substitute in above values and use the Ergun equation to solve for total pressure drop:

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

$$= \frac{150\left(4.10\ * 10^{-7}\frac{lbf-s}{ft^2}\right)(36.5\ ft)(1-0.42)^2}{(0.016\ ft)^2\ * 0.42^3} * 0.591\frac{ft}{s}$$

$$+ \frac{1.75(36.5\ ft)\left(3.67\frac{lb}{ft^3}\right) * \left(\frac{1\ lbf}{32.2\ lbm - \frac{ft}{s^2}}\right)(1-0.42)}{(0.016\ ft) * 0.42^3} * \left(0.591\frac{ft}{s}\right)^2$$

$$= 1231.2\ psf * \frac{ft^2}{144\ in^2} = 8.55\ psi \quad \text{(A20)}$$

$$\Delta P_{section} = \frac{\Delta P_{tot}}{4} = \frac{8.55\ psi}{4} = 2.14\ psi \quad \text{(A21)}$$

Appendix 4.4 Flash Drum Design

Based on thermodynamic results from ASPEN, operating conditions for the flash were chosen to be 110 °F and 145 psig. Average total vapor fraction (VF) of all inlet streams and corresponding vapor and liquid densities (ρ) were used with a vapor velocity design K-factor of 0.27 to determine maximum allowable vapor velocities (u_{vap}) within the drum. After setting an L/D ratio of 3 for a horizontal pressure vessel to minimize equipment space, mass flowrates (m) with a hold-up time of 5 min to allow proper separation, and a liquid level within the tank of 50%, were used to calculate the dimensions of the drum.

Sample Calculations with T-301

$$\frac{L}{D} = 3 \quad \text{(A22)}$$

$$VF_{avg} = \frac{(VF_1 m_1) + (VF_2 m_2)}{m_1 + m_2} = \frac{\left(0.236 * 190454\frac{lb}{hr}\right) + \left(0.007 * 319238\frac{lb}{hr}\right)}{190454\frac{lb}{hr} + 319238\frac{lb}{hr}} = 0.0926 \quad \text{(A23)}$$

$$Liquid\ Fraction\ (LF_{avg}) = 1 - VF_{avg} = 1 - 0.0926 = 0.9074 \quad \text{(A24)}$$

$$u_{vap} = K\sqrt{\frac{\rho_{liq} - \rho_{vap}}{\rho_{vap}}} = 0.27 * \sqrt{\frac{54.9\frac{lb}{ft^3} - 0.772\frac{lb}{ft^3}}{0.772\frac{lb}{ft^3}}} = 2.26\frac{ft}{s} \quad \text{(A25)}$$

$$Volume\ of\ liquid\ held\ (V) = \frac{(m_1 + m_2) * LF_{avg} * holdup}{\rho_{liq}} * \frac{hr}{60\ min}$$

$$= \frac{509692\,\frac{lb}{hr} * 0.9074 * 5\ min}{54.9\,\frac{lb}{ft^3}} * \frac{hr}{60\ min} = 702\ ft^3 \quad \text{(A26)}$$

$$Diameter\ (D) = \left(\frac{4 * V}{frac\ full * \pi * L/D}\right)^{1/3} = \left(\frac{4 * 702\ ft^3}{0.5 * \pi * 3}\right)^{1/3} = 8.41\ ft \quad \text{(A27)}$$

$$L = 3 * D = 3 * 8.41\ ft = 25.2\ ft \quad \text{(A28)}$$

Appendix 4.5 Distillation Column & Reflux Accumulator Design

The operating conditions and design specifications for distillation columns T-302, T-401, and T-402 were taken from ASPEN, with those for the first distillation tower, T-302, chosen to be 389.9 °F and 8.7 psig. The number of theoretical stages required for adequate separation was also determined from ASPEN. Tower T-302 was found to have 12 theoretical stages, or 11 theoretical trays plus the reboiler. The tray profiles for each column provided data on the viscosity of liquid from each stage in centipoise and the K values for the heavy and light keys (phenol and benzene in the first column). The empirical O'Connell relationship[A4.2] relates the liquid viscosity μ_L on each tray with the relative volatility α of the heavy and light components on each tray to determine the Murphree tray efficiencies, E_{OC}, for 90% of efficiency data within +/- 10%.

Reflux accumulators were designed based on the volumetric flowrate of the reflux cycling through. A residence time for each unit was set to 5 minutes with an L/D of 2.

[A4.2] Baburao, Dadasaheb Baburao. *An O'Connell Type Correlation for Prediction of Overall Efficiency of Valve Tray Columns*. Pune, Maharashtra, India: n.p., 2006. Print.

Sample Calculations with T-302 & V-301

$$O'Connell\ Relationship: E_{OC} = 0.492 * (\mu_L \alpha)^{-0.245} \quad \text{(A29)}$$

For Tray 2: *Relative Volatility,* $\alpha_1 = \frac{K_{1,2}}{K_{2,2}} = \frac{0.993521}{0.0799125} = 12.483$ (A30)

$$E_{OC,2} = 0.492 * \left((.2203) * \ 12.48\right)^{-0.245} = 0.384 \quad \text{(A31)}$$

$$Real\ Trays\ Required = \frac{1}{Tray\ Efficiency} = \frac{1}{.384} = 2.62 \quad \text{(A32)}$$

Real Tray Number = $\sum_{i=11} \boldsymbol{Real\ Trays\ Required} = \mathbf{26.02}$ (A33)

Because we cannot purchase a column with 2% of a tray, we must account for 27 total trays in the column according to the efficiency estimates from the O'Connell correlation.

Table A4.1. Summary of hydrodynamic data and tray efficiencies for column T-302.

Theoretical Stage Number	***Viscosity of Liquid from Stage*** μ_L ***(Centipoise)***	***K_2 Value (Phenol)***	***K_1 Value (Benzene)***	***Relative Volatility*** α	***Stage Efficiency*** E_{OC}	***Real Trays Required***	***Real Tray Number***
Condenser1	-	-	-	-	-	-	-
2	0.2206	0.0796	0.9935	12.4830	*0.384*	*2.62*	2.62
3	0.2203	0.0799	0.9950	12.4513	*0.384*	*2.62*	5.24
4	0.2205	0.0802	0.9979	12.4430	*0.384*	*2.62*	7.86
5	0.2221	0.0809	1.0106	12.4979	*0.383*	*2.64*	10.5
6	0.2296	0.0837	1.0698	12.7884	*0.378*	*2.68*	13.18
7	0.2294	0.0843	1.0744	12.7488	*0.378*	*2.68*	15.86
8	0.2319	0.0856	1.0998	12.8447	*0.377*	*2.74*	18.6
9	0.2512	0.1006	1.3843	13.7622	*0.363*	*2.79*	21.39
10	0.1964	0.2976	3.5733	12.0086	*0.399*	*2.56*	23.95
11	0.1179	0.7944	6.7562	8.5052	*0.492*	*2.07*	26.02
Reboiler 12	0.1065	0.9877	7.7546	7.8516	-	-	-
Total							***27***

$$D = \left(\frac{4 * Volummetric\ Reflux\ Flow * Residence\ Time}{\pi}\right)^{1/3} = \left(\frac{4 * 64.6\ \frac{ft^3}{min} * 5\ min}{\pi}\right)^{1/3} = 7.44\ ft \quad \text{(A34)}$$

$$L = 2 * D = 2 * 7.44\ ft = 14.9\ ft \quad \text{(A35)}$$

Appendix 4.6 Storage Tank Considerations

For all four storage tanks, sizing was based on the amount of the feed or product that is desired to be maintained, as well as the volumetric flow ($\dot{V}$) into the three product tanks or the volumetric flow ($\dot{V}$) required from the feed tank. A volumetric safety factor of 1.67 was used to ensure that the tank never operates at full capacity for control and pressure considerations. The dimensions were obtained from setting an L/D ratio of 1. To maintain temperatures of 113 °F for the three heated storage tanks, pump-around heat exchangers are used. Two-inch-thick (t) insulation with a thermal conductivity k of 0.4 BTU-in/(hr-ft^2-°F) is used to estimate the heat lost to the surroundings ($\dot{Q}$) from each of the heated tanks. A 25% error factor was used to account for the assumption that all heat lost is from the insulation to the surroundings. This heat duty was then used to size the heat exchanger itself in the manner described in Appendix 4.2.1, pg. 213. The mass flowrate (m) of the product necessary for the pump-around was determined based on the constant pressure heat capacity c_p of the fluid, as well as the allowable temperature rise from 105 °F to 123 °F in order to maintain an average tank temperature of 113 °F.

Sample Calculations using TK-501

$$Volume\ (V) = Volumetric\ Flow\ (\dot{V}) * \ Time\ capacity * Safety\ Factor$$

$$= 954 \frac{ft^3}{hr} * \frac{24\ hr}{day} * 7\ days * 1.67 = 267{,}588\ ft^3 \tag{A36}$$

$$Diameter\ (D) = \left(\frac{4 * V}{\pi}\right)^{1/3} = \left(\frac{4 * 267{,}588\ ft^3}{\pi}\right)^{1/3} \cong 70\ ft\ \cong Length\ (L) \tag{A37}$$

$$Surface\ Area\ (A) = 2 * \pi * \left(\frac{D}{2}\right)^2 + 2 * \pi * \left(\frac{D}{2}\right) * L$$

$$= 2 * \pi * \left(\frac{70\ ft}{2}\right)^2 + 2 * \pi * \left(\frac{70\ ft}{2}\right) * 70\ ft = 22{,}988\ ft^2 \quad \text{(A38)}$$

$$Heat\ Lost\ (\dot{Q}) = \frac{k * A * \Delta T * Error\ Factor}{t}$$

$$= \frac{0.4 \frac{BTU - in}{hr - ft^2 - °\text{F}} * 22{,}988\ ft^2 * (113\ °\text{F} - 86°\text{F}) * 1.25}{2\ in} \quad \text{(A39)}$$

$$= 155{,}166 \frac{BTU}{hr}$$

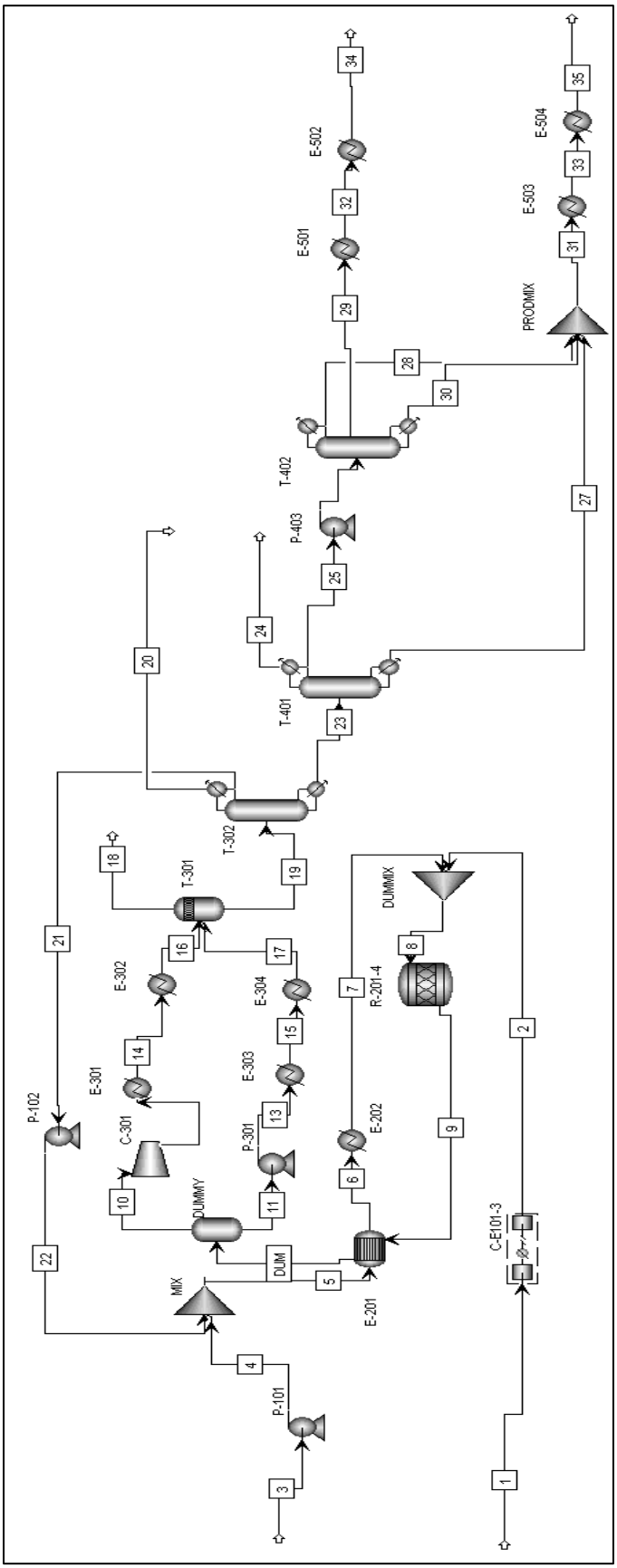
$$Pumparound\ Flow\ (m) = \frac{\dot{Q} * MW}{c_p * \Delta T} = \frac{155{,}166 \frac{BTU}{hr} * 94.13 \frac{lb}{lbmol}}{40.12 \frac{BTU}{lbmol - °\text{F}} * (123\ °\text{F} - 105\ °\text{F})}$$

$$= 20{,}226\ lb/hr \quad \text{(A40)}$$

Appendix 5

ASPEN Process Simulation

Appendix 5.1: Process Flowsheet



Appendix 5.2: Input File

```
;
;Input Summary created by ASPEN Plus Rel. 35.0 at 11:18:25 Thu Apr 6, 2017
;Directory S:\Documents\459\WORKING  Filename C:\Users\rtann\AppData\Local\Temp\~ap5829.txt
;


DYNAMICS
   DYNAMICS RESULTS=ON

IN-UNITS ENG SHORT-LENGTH=in

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES PEQ-CHK-FRAC=1E-015  &
       MASS-BAL-TOL=0.0001

MODEL-OPTION

DATABANKS 'APV90 PURE35' / 'APV90 AQUEOUS' / 'APV90 SOLIDS' /  &
       'APV90 INORGANIC' / 'APEOSV90 AP-EOS' /  &
       'NISTV90 NIST-TRC' / NOASPENPCD

PROP-SOURCES 'APV90 PURE35' / 'APV90 AQUEOUS' / 'APV90 SOLIDS' &
        / 'APV90 INORGANIC' / 'APEOSV90 AP-EOS' /  &
       'NISTV90 NIST-TRC'

COMPONENTS
   BENZENE C6H6 /
   PHENOL C6H6O /
   CATECHOL C6H6O2-E1 /
   BENZO-01 C7H6O2 /
   BENZA-01 C7H6O /
   WATER H2O /
   OXYGEN O2 /
   NITROGEN N2

HENRY-COMPS HC-1 OXYGEN NITROGEN

SOLVE
   PARAM SEPSEQ=NO
   RUN-MODE MODE=SIM

FLOWSHEET
   BLOCK T-302 IN=19 OUT=20 21 23
   BLOCK T-301 IN=17 16 OUT=18 19
   BLOCK R-201-4 IN=8 OUT=9
   BLOCK MIX IN=22 4 OUT=5
   BLOCK E-201 IN=9 5 OUT=DUM 6
   BLOCK E-202 IN=6 OUT=7
   BLOCK E-304 IN=15 OUT=17
   BLOCK P-102 IN=21 OUT=22
   BLOCK P-101 IN=3 OUT=4
```

```
   BLOCK C-E101-3 IN=1 OUT=2
   BLOCK DUMMY IN=DUM OUT=10 11
   BLOCK E-302 IN=14 OUT=16
   BLOCK T-401 IN=23 OUT=24 25 27
   BLOCK DUMMIX IN=2 7 OUT=8
   BLOCK E-502 IN=32 OUT=34
   BLOCK E-504 IN=33 OUT=35
   BLOCK C-301 IN=10 OUT=12
   BLOCK P-301 IN=11 OUT=13
   BLOCK E-301 IN=12 OUT=14
   BLOCK E-303 IN=13 OUT=15
   BLOCK T-402 IN=26 OUT=28 30 29
   BLOCK P-403 IN=25 OUT=26
   BLOCK PRODMIX IN=30 27 28 OUT=31
   BLOCK E-501 IN=29 OUT=32
   BLOCK E-503 IN=31 OUT=33

PROPERTIES PENG-ROB
   PROPERTIES NRTL

ESTIMATE ALL
   NRTL ALL ALL UNIFAC

PROP-DATA HENRY-1
   IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
      INVERSE-PRES='1/bar' SHORT-LENGTH=mm
   PROP-LIST HENRY
   BPVAL OXYGEN BENZENE 21.67187354 -437.4599910 -2.341200000  &
      8.72000000E-4 10.00000000 60.00000000 0.0
   BPVAL OXYGEN WATER 144.4080745 -7775.060000 -18.39740000  &
      -9.4435400E-3 .8500000000 74.85000000 0.0
   BPVAL NITROGEN BENZENE -62.53052646 1916.800049 12.54900000  &
      -.0257110000 7.100000000 60.00000000 0.0
   BPVAL NITROGEN WATER 164.9940745 -8432.770000 -21.55800000  &
      -8.4362400E-3 -.1500000000 72.85000000 0.0

PROP-DATA NRTL-1
   IN-UNITS MET PRESSURE=bar TEMPERATURE=C DELTA-T=C PDROP=bar  &
      INVERSE-PRES='1/bar' SHORT-LENGTH=mm
   PROP-LIST NRTL
   BPVAL BENZENE PHENOL 0.0 389.2036000 .3000000000 0.0 0.0  &
      0.0 70.00000000 80.00000000
   BPVAL PHENOL BENZENE 0.0 -15.05350000 .3000000000 0.0 0.0  &
      0.0 70.00000000 80.00000000
   BPVAL BENZENE WATER 45.19050000 591.3676000 .2000000000 0.0  &
      -7.562900000 0.0 .8000000000 77.00000000
   BPVAL WATER BENZENE 140.0874000 -5954.307100 .2000000000  &
      0.0 -20.02540000 0.0 .8000000000 77.00000000
   BPVAL PHENOL BENZA-01 0.0 356.6832000 .3000000000 0.0 0.0  &
      0.0 115.1500000 122.2000000
   BPVAL BENZA-01 PHENOL 0.0 -449.1747000 .3000000000 0.0 0.0  &
      0.0 115.1500000 122.2000000
   BPVAL PHENOL WATER 2.301500000 -879.7008000 .3000000000 0.0  &
      0.0 0.0 44.40000000 182.0000000
```

```
BPVAL WATER PHENOL -.5363000000 1412.731600 .3000000000 0.0  &
   0.0 0.0 44.40000000 182.0000000
BPVAL BENZO-01 WATER 253.4649000 -9663.475600 .2000000000  &
   0.0 -38.85230000 0.0 64.00000000 115.5000000
BPVAL WATER BENZO-01 507.4191000 -27731.77730 .2000000000  &
   0.0 -71.92100000 0.0 64.00000000 115.5000000
BPVAL PHENOL BENZO-01 0.0 439.3573100 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZO-01 PHENOL 0.0 -185.5319200 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZO-01 BENZA-01 0.0 -193.2510240 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZA-01 BENZO-01 0.0 420.6283360 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZA-01 WATER 0.0 839.3810740 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL WATER BENZA-01 0.0 1752.355170 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZENE CATECHOL 0.0 1509.274030 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL CATECHOL BENZENE 0.0 -3.561853730 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZENE BENZO-01 0.0 555.4487960 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZO-01 BENZENE 0.0 -141.1490830 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZENE BENZA-01 0.0 296.0398560 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZA-01 BENZENE 0.0 -132.1842970 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZENE OXYGEN 0.0 805.1484280 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL OXYGEN BENZENE 0.0 -533.1209200 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL BENZENE NITROGEN 0.0 729.0478970 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL NITROGEN BENZENE 0.0 -497.2678470 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL PHENOL CATECHOL 0.0 163.0115060 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL CATECHOL PHENOL 0.0 -93.15335030 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL PHENOL OXYGEN 0.0 -429.9818290 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL OXYGEN PHENOL 0.0 128.3592970 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL PHENOL NITROGEN 0.0 -387.4383670 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL NITROGEN PHENOL 0.0 74.60129170 .3000000000 0.0 0.0  &
   0.0 25.00000000 25.00000000
BPVAL CATECHOL BENZO-01 0.0 382.6082020 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
BPVAL BENZO-01 CATECHOL 0.0 -6.899688710 .3000000000 0.0  &
   0.0 0.0 25.00000000 25.00000000
```

```
   BPVAL CATECHOL BENZA-01 0.0 -347.3339800 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL BENZA-01 CATECHOL 0.0 35.24558880 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL CATECHOL OXYGEN 0.0 2030.082890 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL OXYGEN CATECHOL 0.0 -920.7941860 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL CATECHOL WATER 0.0 2139.798090 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL WATER CATECHOL 0.0 -904.1092180 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL CATECHOL NITROGEN 0.0 1899.822030 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL NITROGEN CATECHOL 0.0 -892.5357340 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL BENZO-01 OXYGEN 0.0 2413.743770 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL OXYGEN BENZO-01 0.0 -997.3756170 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL BENZO-01 NITROGEN 0.0 2220.857730 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL NITROGEN BENZO-01 0.0 -959.6016860 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL BENZA-01 OXYGEN 0.0 1804.820110 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL OXYGEN BENZA-01 0.0 -860.9135230 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL BENZA-01 NITROGEN 0.0 1670.272620 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL NITROGEN BENZA-01 0.0 -827.3024430 .3000000000 0.0  &
      0.0 0.0 25.00000000 25.00000000
   BPVAL OXYGEN WATER 0.0 182.2724850 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL WATER OXYGEN 0.0 -107.2436390 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL OXYGEN NITROGEN 0.0 4.268334610 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL NITROGEN OXYGEN 0.0 -5.121252420 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL WATER NITROGEN 0.0 -35.82780730 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000
   BPVAL NITROGEN WATER 0.0 142.4194540 .3000000000 0.0 0.0  &
      0.0 25.00000000 25.00000000

PROP-DATA PRKBV-1
   IN-UNITS ENG SHORT-LENGTH=in
   PROP-LIST PRKBV
   BPVAL BENZENE NITROGEN .1641000000 0.0 0.0 -459.6700000  &
      1340.330000
   BPVAL NITROGEN BENZENE .1641000000 0.0 0.0 -459.6700000  &
      1340.330000
   BPVAL OXYGEN NITROGEN -.0119000000 0.0 0.0 -459.6700000  &
      1340.330000
```

```
   BPVAL NITROGEN OXYGEN -.0119000000 0.0 0.0 -459.6700000  &
      1340.330000

STREAM 1
   SUBSTREAM MIXED TEMP=30. <C> PRES=14.7
   MOLE-FLOW OXYGEN 410. / NITROGEN 1551.133

STREAM 3
   SUBSTREAM MIXED TEMP=30. <C> PRES=14.7
   MOLE-FLOW BENZENE 840.

STREAM 21
   SUBSTREAM MIXED TEMP=240. PRES=50.
   MOLE-FLOW BENZENE 2000.

STREAM 22
   SUBSTREAM MIXED TEMP=245. PRES=4.4 <MPag>
   MOLE-FLOW BENZENE 6000. / PHENOL 1.36 / OXYGEN 1. /  &
      NITROGEN 8.

BLOCK DUMMIX MIXER
   PARAM

BLOCK MIX MIXER
   PARAM

BLOCK PRODMIX MIXER
   PARAM

BLOCK E-202 HEATER
   PARAM TEMP=370. <C> PRES=-5. DPPARMOPT=NO

BLOCK E-301 HEATER
   PARAM TEMP=285. PRES=-5. DPPARMOPT=NO

BLOCK E-302 HEATER
   PARAM TEMP=110. PRES=-5. DPPARMOPT=NO

BLOCK E-303 HEATER
   PARAM TEMP=285. PRES=-5. DPPARMOPT=NO

BLOCK E-304 HEATER
   PARAM TEMP=110. PRES=-5. DPPARMOPT=NO

BLOCK E-501 HEATER
   PARAM TEMP=285. PRES=-5. DPPARMOPT=NO

BLOCK E-502 HEATER
   PARAM TEMP=45. <C> PRES=-5. DPPARMOPT=NO

BLOCK E-503 HEATER
   PARAM TEMP=285. PRES=-5. DPPARMOPT=NO

BLOCK E-504 HEATER
```

```
   PARAM TEMP=45. <C> PRES=-5. DPPARMOPT=NO

BLOCK DUMMY FLASH2
   PARAM PRES=0. DUTY=0.

BLOCK T-301 FLASH2
   PARAM PRES=0. <bar> DUTY=0.

BLOCK E-201 HEATX
   PARAM CALC-TYPE=SIMULATION CALC-METHOD=TASCPLUS-RIG
   HETRAN-PARAM INPUT-FILE= &
   'E-201_1.edr' SAV-INPUT=YES
   FEEDS HOT=9 COLD=5
   OUTLETS-HOT DUM
   OUTLETS-COLD 6
   FLASH-SPECS DUM MAXIT=100
   FLASH-SPECS 6 MAXIT=100
   HOT-SIDE SHELL-TUBE=TUBE DPPARMOPT=NO
   COLD-SIDE DPPARMOPT=NO
   TQ-PARAM CURVE=YES

BLOCK T-302 RADFRAC
   SUBOBJECTS INTERNALS = CS-1 CS-2
   PARAM NSTAGE=12 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=200  &
      TOLOL=0.0001 DAMPING=NONE
   PARAM2 STATIC-DP=YES
   COL-CONFIG CONDENSER=PARTIAL-V-L REBOILER=KETTLE  &
      CA-CONFIG=INT-1
   FEEDS 19 6
   PRODUCTS 20 1 V / 21 1 L / 23 12 L
   P-SPEC 1 20.
   COL-SPECS DP-STAGE=0.14 MOLE-RDV=0.02 MOLE-B=740.  &
      MOLE-RR=0.5 DP-COND=2.
   SPEC 3 MOLE-FRAC 0.005 COMPS=BENZENE STREAMS=23
   VARY 3 MOLE-B 500. 1000.
   REPORT NOHYDRAULIC
   INTERNALS CS-1 STAGE1=2 STAGE2=5 P-UPDATE=NO NPASS=4  &
      TRAY-SPACE=1.5
   TRAY-SIZE 1 2 5 SIEVE
   INTERNALS CS-2 STAGE1=6 STAGE2=11 P-UPDATE=NO  &
      TRAY-SPACE=1.5
   TRAY-SIZE 2 6 11 SIEVE

BLOCK T-401 RADFRAC
   SUBOBJECTS INTERNALS = CS-1 CS-2
   PARAM NSTAGE=12 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=25  &
      DAMPING=NONE
   PARAM2 STATIC-DP=YES
   COL-CONFIG CONDENSER=PARTIAL-V-L CA-CONFIG=INT-1
   FEEDS 23 6 ON-STAGE
   PRODUCTS 24 1 V / 25 1 L / 27 12 L
   P-SPEC 1 20.
   COL-SPECS DP-STAGE=0.15 MOLE-RDV=0.01 MOLE-D=703. MOLE-RR=4.  &
      DP-COND=2.
```

```
   REPORT NOHYDRAULIC
   INTERNALS CS-1 STAGE1=2 STAGE2=5 P-UPDATE=NO NPASS=2  &
      TRAY-SPACE=1.5
   TRAY-SIZE 1 2 5 SIEVE
   INTERNALS CS-2 STAGE1=6 STAGE2=11 P-UPDATE=NO NPASS=2  &
      TRAY-SPACE=1.5
   TRAY-SIZE 2 6 11 SIEVE

BLOCK T-402 RADFRAC
   SUBOBJECTS INTERNALS = CS-1 CS-2
   PARAM NSTAGE=20 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=25  &
      DAMPING=NONE
   PARAM2 STATIC-DP=YES
   COL-CONFIG CONDENSER=TOTAL CA-CONFIG=INT-1
   FEEDS 26 15
   PRODUCTS 30 20 L / 29 18 V MOLE-FLOW=672. / 28 1 L
   P-SPEC 1 20.
   COL-SPECS DP-STAGE=0.15 MOLE-D=23.5 MOLE-RR=20. DP-COND=2.
   SPEC 1 MASS-FRAC 0.9983 COMPS=PHENOL STREAMS=29  &
      SPEC-ACTIVE=YES
   VARY 1 MOLE-RR 1. 1000. VARY-ACTIVE=YES
   REPORT NOHYDRAULIC
   INTERNALS CS-1 STAGE1=2 STAGE2=14 P-UPDATE=NO NPASS=2  &
      TRAY-SPACE=1.5
   TRAY-SIZE 1 2 14 SIEVE
   INTERNALS CS-2 STAGE1=15 STAGE2=19 P-UPDATE=NO NPASS=2  &
      TRAY-SPACE=1.5
   TRAY-SIZE 2 15 19 SIEVE

BLOCK R-201-4 RSTOIC
   PARAM TEMP=350. <C> PRES=4. <MPag> MAXIT=100 TOL=0.0001  &
      HEAT-OF-REAC=YES COMBUSTION=NO
   STOIC 1 MIXED BENZENE -1. / OXYGEN -0.5 / PHENOL 1.
   STOIC 2 MIXED BENZENE -7. / OXYGEN -7.5 / BENZO-01 6. /  &
      WATER 3.
   STOIC 3 MIXED BENZENE -7. / OXYGEN -4.5 / BENZA-01 6. /  &
      WATER 3.
   STOIC 4 MIXED BENZENE -1. / OXYGEN -1. / CATECHOL 1.
   CONV 1 MIXED BENZENE 0.121
   CONV 2 MIXED BENZENE 0.00025
   CONV 3 MIXED BENZENE 0.00025
   CONV 4 MIXED BENZENE 0.0035
   HEAT-RXN REACNO=1 CID=BENZENE / REACNO=2 CID=BENZENE /  &
      REACNO=3 CID=BENZENE / REACNO=4 CID=BENZENE

BLOCK P-101 PUMP
   PARAM PRES=4.4 <MPag>

BLOCK P-102 PUMP
   PARAM PRES=4.4 <MPag> NPHASE=2 MAXIT=100
   BLOCK-OPTION FREE-WATER=NO

BLOCK P-301 PUMP
   PARAM PRES=155.04 <psig> EFF=0.6 PUMP-TYPE=TURBINE
```

```
BLOCK P-403 PUMP
   PARAM PRES=30.

BLOCK C-301 COMPR
   PARAM TYPE=ASME-ISENTROP PRES=155.04 <psig> SEFF=0.85  &
      MEFF=0.98 NPHASE=2 SB-MAXIT=30 SB-TOL=0.0001   &
      MODEL-TYPE=TURBINE
   BLOCK-OPTION FREE-WATER=NO

BLOCK C-E101-3 MCOMPR
   PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=4. <MPag> SB-MAXIT=30  &
      SB-TOL=0.0001
   FEEDS 1 1
   PRODUCTS 2 3
   COMPR-SPECS 1 SEFF=0.85 MEFF=1. / 2 SEFF=0.85 MEFF=1. /  &
      3 SEFF=0.85 MEFF=1.
   COOLER-SPECS 1 TEMP=100. PDROP=5. / 2 TEMP=100. PDROP=5. /  &
      3 DUTY=0.

UTILITY U-1 GENERAL
   DESCRIPTION "Cooling Water, Inlet Temp=20 C, Outlet Temp=25 C"
   COST ENERGY-PRICE=2.12E-007 <$/kJ>
   PARAM UTILITY-TYPE=WATER PRES=1. <atm> PRES-OUT=1. <atm>  &
      TIN=20. <C> TOUT=25. <C> CALOPT=FLASH MIN-TAPP=5. <C>  &
      HTC=0.0135 <GJ/hr-sqm-C>

DESIGN-SPEC DS-1
   DEFINE PROD MOLE-FLOW STREAM=23 SUBSTREAM=MIXED  &
      COMPONENT=PHENOL UOM="lbmol/hr"
   SPEC "PROD" TO "680"
   TOL-SPEC "0.1"
   VARY MOLE-FLOW STREAM=3 SUBSTREAM=MIXED COMPONENT=BENZENE  &
      UOM="lbmol/hr"
   LIMITS "840" "870"

EO-CONV-OPTI

CONV-OPTIONS
   WEGSTEIN MAXIT=1000

STREAM-REPOR MOLEFLOW MASSFLOW STDVOLFLOW

PROPERTY-REP PARAMS PCES

DISABLE
   DESIGN-SPEC DS-1
;
;
;
;
```

Appendix 5.3: Block Reports

```
BLOCK:  C-301    MODEL: COMPR
------------------------------
  INLET STREAM:          10
  OUTLET STREAM:         12
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)          3380.95          3380.95          0.00000
      MASS(LB/HR   )           190454.          190454.        0.152813E-15
      ENTHALPY(BTU/HR  )     0.779279E+08     0.705083E+08     0.952100E-01

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

                        ***  INPUT DATA  ***

  ISENTROPIC COMPRESSOR USING ASME METHOD
   OUTLET PRESSURE  PSIA                                  169.736
   ISENTROPIC EFFICIENCY                                  0.85000
   MECHANICAL EFFICIENCY                                  0.98000

                        ***  RESULTS  ***

   INDICATED  HORSEPOWER REQUIREMENT  HP              -2,915.98
   BRAKE      HORSEPOWER REQUIREMENT  HP              -2,857.66
   NET WORK REQUIRED                  HP              -2,857.66
   POWER LOSSES                       HP                  58.3195
   ISENTROPIC HORSEPOWER REQUIREMENT  HP              -2,478.58
   CALCULATED OUTLET TEMP  F                             327.490
   ISENTROPIC TEMPERATURE  F                             332.391
   EFFICIENCY (POLYTR/ISENTR) USED                        0.85000
   OUTLET VAPOR FRACTION                                  0.96622
   HEAD DEVELOPED,       FT-LBF/LB                   -25,767.9
   MECHANICAL EFFICIENCY USED                             0.98000
   INLET HEAT CAPACITY RATIO                              1.19745
```

```
   INLET VOLUMETRIC FLOW RATE , CUFT/HR                47,367.7
   OUTLET VOLUMETRIC FLOW RATE, CUFT/HR               152,629.
   INLET  COMPRESSIBILITY FACTOR                         0.85529
   OUTLET COMPRESSIBILITY FACTOR                         0.90709
   AV. ISENT. VOL. EXPONENT                              1.04459
   AV. ISENT. TEMP EXPONENT                              1.11547
   AV. ACTUAL VOL. EXPONENT                              1.06532
   AV. ACTUAL TEMP EXPONENT                              1.12170

BLOCK:  C-E101-3 MODEL: MCOMPR
------------------------------
  INLET STREAMS:    1            TO STAGE   1
  OUTLET STREAMS:   2          FROM STAGE   3
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            1961.13          1961.13          0.00000
      MASS(LB/HR   )            56572.1          56572.1          0.00000
      ENTHALPY(BTU/HR  )        116355.        0.414967E+07     -0.971960

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

                         ***  INPUT DATA  ***

  ISENTROPIC CENTRIFUGAL COMPRESSOR
  NUMBER OF STAGES                                        3
  FINAL PRESSURE, PSIA                                594.847
  DISTRIBUTION AMONG STAGES                            EQUAL P-RATIO

                  COMPRESSOR SPECIFICATIONS PER STAGE

  STAGE                    MECHANICAL      ISENTROPIC
  NUMBER                   EFFICIENCY      EFFICIENCY
```

1	1.000	0.8500
2	1.000	0.8500
3	1.000	0.8500

COOLER SPECIFICATIONS PER STAGE

STAGE NUMBER	PRESSURE DROP PSI	COOLER SPECIFICATION		
1	5.000	OUTLET TEMPERATURE	100.0	F
2	5.000	OUTLET TEMPERATURE	100.0	F
3	5.000	HEAT DUTY	0.000	BTU/HR

*** RESULTS ***

FINAL PRESSURE, PSIA	594.847
TOTAL WORK REQUIRED, HP	4,628.23
TOTAL COOLING DUTY , BTU/HR	-7,742,920.

*** PROFILE ***

COMPRESSOR PROFILE

STAGE NUMBER	OUTLET PRESSURE PSIA	PRESSURE RATIO	OUTLET TEMPERATURE F
1	50.47	3.433	354.6
2	173.3	3.811	403.1
3	594.8	3.535	384.0

STAGE NUMBER	INDICATED HORSEPOWER HP	BRAKE HORSEPOWER HP
1	1452.	1452.
2	1641.	1641.
3	1535.	1535.

STAGE NUMBER	HEAD DEVELOPED FT-LBF/LB	VOLUMETRIC FLOW CUFT/HR	ISENTROPIC EFFICIENCY

```
    1       0.4319E+05     0.7808E+06     0.8500
    2       0.4883E+05     0.2587E+06     0.8500
    3       0.4567E+05     0.6970E+05     0.8500

                          COOLER PROFILE

  STAGE      OUTLET          OUTLET       COOLING      VAPOR
  NUMBER     TEMPERATURE     PRESSURE     LOAD         FRACTION
             F               PSIA         BTU/HR

    1         100.0           45.47       -.3515E+07   1.000
    2         100.0           168.3       -.4228E+07   1.000
    3         384.0           594.8        0.000       1.000

BLOCK:  DUMMIX   MODEL: MIXER
------------------------------
  INLET STREAMS:          2           7
  OUTLET STREAM:          8
  PROPERTY OPTION SET:    PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            7774.83          7774.83         0.00000
      MASS(LB/HR    )           509692.          509692.         0.00000
      ENTHALPY(BTU/HR  )      0.309315E+09     0.309315E+09      0.00000

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

                          ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  DUMMY    MODEL: FLASH2
------------------------------
```

```
INLET STREAM:          DUM
OUTLET VAPOR STREAM:   10
OUTLET LIQUID STREAM:  11
PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                  ***  MASS AND ENERGY BALANCE  ***
                              IN               OUT        RELATIVE DIFF.
 TOTAL BALANCE
    MOLE(LBMOL/HR)          7402.19          7402.19          0.00000
    MASS(LB/HR    )          509692.          509692.        0.228403E-15
    ENTHALPY(BTU/HR  )    0.162189E+09     0.162189E+09    -0.167809E-08

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

                      ***  INPUT DATA  ***
TWO    PHASE  PQ  FLASH
PRESSURE DROP         PSI                              0.0
SPECIFIED HEAT DUTY   BTU/HR                           0.0
MAXIMUM NO. ITERATIONS                                30
CONVERGENCE TOLERANCE                                  0.000100000

                      ***  RESULTS  ***
OUTLET TEMPERATURE    F                                441.48
OUTLET PRESSURE       PSIA                             590.37
VAPOR FRACTION                                        0.45675


V-L PHASE EQUILIBRIUM :

   COMP            F(I)         X(I)         Y(I)         K(I)
   BENZENE       0.68521      0.81742      0.52796      0.64588
   PHENOL        0.94756E-01  0.15132      0.27477E-01  0.18158
   CATECHOL      0.27408E-02  0.47133E-02  0.39486E-03  0.83775E-01
   BENZO-01      0.16781E-03  0.29621E-03  0.15086E-04  0.50930E-01
   BENZA-01      0.16781E-03  0.27247E-03  0.43326E-04  0.15901
   WATER         0.22761E-02  0.20089E-02  0.25940E-02   1.2913
```

```
     OXYGEN            0.49641E-02    0.80237E-03    0.99141E-02     12.356
     NITROGEN          0.20972        0.23162E-01    0.43160         18.634

BLOCK:  E-201    MODEL: HEATX
------------------------------
  THIS BLOCK RUNS WITH ASPEN EDR 35.0  WITH ADVANCED METHOD FOR SHELL&TUBE
  HOT SIDE:
  ---------
  INLET STREAM:             9
  OUTLET STREAM:            DUM
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE
  COLD SIDE:
  ----------
  INLET STREAM:             5
  OUTLET STREAM:            6
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE


    **************************************************************************
    *                                                                        *
    *     A POTENTIAL TUBE VIBRATIEON PROBLEM IS INDICATED                   *
    *                                                                        *
    **************************************************************************


                     ***  MASS AND ENERGY BALANCE  ***
                                    IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            13215.9          13215.9          0.00000
      MASS(LB/HR    )           962812.          962812.          0.00000
      ENTHALPY(BTU/HR  )     0.389799E+09     0.389799E+09     0.152911E-15

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

                          ***  INPUT DATA  ***

  FLASH SPECS FOR HOT SIDE:
```

```
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                  100
CONVERGENCE TOLERANCE                                    0.000100000

FLASH SPECS FOR COLD SIDE:
TWO    PHASE      FLASH
MAXIMUM NO. ITERATIONS                                  100
CONVERGENCE TOLERANCE                                    0.000100000

SHELL&TUBE INPUT FILE NAME                                    E-201_1.EDR
SHELL&TUBE PROGRAM MODE                                       SIMULATION

HEAT CURVE GENERATION
  HOT  HEAT CURVE GENERATED BY                            ASPEN PLUS
  COLD HEAT CURVE GENERATED BY                            ASPEN PLUS

                      ***  OVERALL RESULTS  ***

STREAMS:
                 ---------------------------------------
                 |                                     |
9          ----->|            HOT  (TUBE)              |-----> DUM
T=  6.6200D+02   |                                     |       T=  4.4148D+02
P=  5.9485D+02   |                                     |       P=  5.9037D+02
V=  1.0000D+00   |                                     |       V=  4.5675D-01
                 |                                     |
6          <-----|            COLD (SHELL)             |<----- 5
T=  5.1540D+02   |                                     |       T=  1.6503D+02
P=  6.5113D+02   |                                     |       P=  6.5286D+02
V=  0.0000D+00   |                                     |       V=  0.0000D+00
                 ---------------------------------------

UNIT RESULTS:
  CALCULATED HEAT DUTY          BTU/HR          88350259.4085
  CALCULATED (REQUIRED) AREA    SQFT                8474.9770
  ACTUAL EXCHANGER AREA         SQFT                8401.4600
  % OVER (UNDER) DESIGN                               -0.8675
  AVERAGE COEFFICIENT           BTU/HR-SQFT-R         84.9222
  UA                            BTU/HR-R            719713.9569
  LMTD (CORRECTED)              F                   122.7575
  LMTD CORRECTION FACTOR                              0.5601
  NUMBER OF SHELLS IN SERIES                             1
```

```
    NUMBER OF SHELLS IN PARALLEL                          1
    HIGH RHOV2 INDICATION                                NO
    VIBRATION INDICATION                                 YES

  SHELLSIDE RESULTS:
    MEAN SHELL METAL TEMPERATURE      F                382.0101
    TOTAL PRESSURE DROP               PSI                1.7321
    WINDOW PRESSURE DROP              PSI                0.2471
    CROSSFLOW PRESSURE DROP           PSI                1.0877
    BULK FILM COEFFICIENT             BTU/HR-SQFT-R    308.4036
    WALL FILM COEFFICIENT             BTU/HR-SQFT-R    308.4036
    THERMAL RESISTANCE                HR-SQFT-R/BTU      0.0032
    MAXIMUM FOULING RESISTANCE        HR-SQFT-R/BTU    0.001954
    FOULING RESISTANCE                HR-SQFT-R/BTU      0.0020
    CROSSFLOW VELOCITY                FT/SEC             3.1535
    WINDOW VELOCITY                   FT/SEC             3.7280
    MIDPOINT VELOCITY                 FT/SEC             3.4408
    SHELL ENTRANCE RHOV^2             LB/FT-SQSEC      519.2851
    SHELL EXIT RHOV^2                 LB/FT-SQSEC      616.4698
    BUNDLE ENTRANCE RHOV^2            LB/FT-SQSEC      395.5520
    BUNDLE EXIT RHOV^2                LB/FT-SQSEC       41.3808
    FOULING % OF OVERALL RESISTANCE                     16.9852
    FILM % OF OVERALL RESISTANCE                        27.5361
    FRICTIONAL PRESSURE DROP          PSI                1.7404

  TUBESIDE RESULTS:
    MEAN TUBE METAL TEMPERATURE       F                440.4560
    TOTAL PRESSURE DROP               PSI                4.4793
    BULK FILM COEFFICIENT             BTU/HR-SQFT-R    285.3572
    WALL FILM COEFFICIENT             BTU/HR-SQFT-R    285.3572
    THERMAL RESISTANCE                HR-SQFT-R/BTU      0.0035
    MAXIMUM FOULING RESISTANCE        HR-SQFT-R/BTU    0.002364
    FOULING RESISTANCE                HR-SQFT-R/BTU      0.0024
    INPUT VELOCITY                    FT/SEC            24.1949
    OUTLET VELOCITY                   FT/SEC            10.4619
    FOULING % OF OVERALL RESISTANCE                     20.5467
    FILM % OF OVERALL RESISTANCE                        29.7600
    FRICTIONAL PRESSURE DROP          PSI                4.8114

HEATX COLD-TQCU E-201    TQCURV INLET
-------------------------------------
  PRESSURE PROFILE:      CONSTANT2
```

PRESSURE DROP: -1.7321 PSI
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

DUTY	PRES	TEMP	VFRAC
BTU/HR	PSIA	F	
0.0	652.8620	515.4622	0.0
4.2072+06	652.8620	504.5895	0.0
8.4143+06	652.8620	492.7799	0.0
1.2621+07	652.8620	480.1943	0.0
1.6829+07	652.8620	466.9420	0.0
2.1036+07	652.8620	453.0988	0.0
2.5243+07	652.8620	438.7180	0.0
2.9450+07	652.8620	423.8369	0.0
3.3657+07	652.8620	408.4809	0.0
3.7754+07	652.8620	393.0883	0.0
3.7864+07	652.8620	392.6664	0.0
4.2072+07	652.8620	376.4021	0.0
4.6279+07	652.8620	359.6909	0.0
5.0486+07	652.8620	342.5300	0.0
5.4693+07	652.8620	324.9117	0.0
5.8900+07	652.8620	306.8238	0.0
6.3107+07	652.8620	288.2493	0.0
6.7314+07	652.8620	269.1667	0.0
7.1522+07	652.8620	249.5496	0.0
7.5729+07	652.8620	229.3666	0.0
7.9936+07	652.8620	208.5812	0.0
8.4143+07	652.8620	187.1514	0.0
8.8350+07	652.8620	165.0295	0.0

HEATX HOT-TQCUR E-201 TQCURV INLET

```
  PRESSURE PROFILE:       CONSTANT2
  PRESSURE DROP:          0.0          PSI
  PROPERTY OPTION SET:    PENG-ROB   STANDARD PR EQUATION OF STATE
```

DUTY	PRES	TEMP	VFRAC
BTU/HR	PSIA	F	
0.0	594.8469	662.0000	1.0000
4.2072+06	594.8469	645.8641	1.0000
8.4143+06	594.8469	629.6639	1.0000
1.2621+07	594.8469	613.4054	1.0000
1.6829+07	594.8469	597.0968	1.0000
2.1036+07	594.8469	580.7490	1.0000
2.5243+07	594.8469	564.3767	1.0000
2.9450+07	594.8469	547.9998	1.0000
3.3657+07	594.8469	531.6449	1.0000
3.7754+07	594.8469	515.7760	DEW>1.0000
3.7864+07	594.8469	515.6388	0.9987
4.2072+07	594.8469	510.4240	0.9489
4.6279+07	594.8469	505.1802	0.8987
5.0486+07	594.8469	499.8691	0.8484
5.4693+07	594.8469	494.4507	0.7985
5.8900+07	594.8469	488.8827	0.7492
6.3107+07	594.8469	483.1203	0.7011
6.7314+07	594.8469	477.1171	0.6546
7.1522+07	594.8469	470.8260	0.6099
7.5729+07	594.8469	464.2006	0.5673
7.9936+07	594.8469	457.1963	0.5272
8.4143+07	594.8469	449.7716	0.4897
8.8350+07	594.8469	441.8891	0.4550

```
BLOCK:  E-202    MODEL: HEATER
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  INLET STREAM:          6
  OUTLET STREAM:         7
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN                OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           5813.70          5813.70          0.00000
      MASS(LB/HR    )           453120.          453120.          0.00000
      ENTHALPY(BTU/HR  )     0.227610E+09     0.305165E+09    -0.254142

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

                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE                F                       698.000
  PRESSURE DROP                        PSI                       5.00000
  MAXIMUM NO. ITERATIONS                                        30
  CONVERGENCE TOLERANCE                                          0.000100000


                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                     698.00
  OUTLET PRESSURE       PSIA                                  646.13
  HEAT DUTY             BTU/HR                              0.77555E+08
  OUTLET VAPOR FRACTION                                       1.0000


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     BENZENE       0.99706       0.99764       0.99706       1.4901
     PHENOL        0.18287E-05   0.21855E-05   0.18287E-05   1.2475
     CATECHOL      0.39874E-11   0.52066E-11   0.39874E-11   1.1418
```

BENZO-01	0.24312E-14	0.36511E-14	0.24312E-14	0.99278
BENZA-01	0.33990E-08	0.43684E-08	0.33990E-08	1.1601
WATER	0.26841E-02	0.22169E-02	0.26841E-02	1.8051
OXYGEN	0.36872E-04	0.21451E-04	0.36872E-04	2.5627
NITROGEN	0.21240E-03	0.11575E-03	0.21240E-03	2.7359

BLOCK: E-301 MODEL: HEATER

INLET STREAM: 12
OUTLET STREAM: 14
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	3380.95	3380.95	0.00000
MASS(LB/HR)	190454.	190454.	0.00000
ENTHALPY(BTU/HR)	0.705083E+08	0.588878E+08	0.164812

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	F	285.000
PRESSURE DROP	PSI	5.00000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	F	285.00
OUTLET PRESSURE	PSIA	164.74
HEAT DUTY	BTU/HR	-0.11621E+08
OUTLET VAPOR FRACTION		0.74835

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
BENZENE	0.52796	0.89473	0.40463	0.45223
PHENOL	0.27477E-01	0.96101E-01	0.44005E-02	0.45790E-01
CATECHOL	0.39486E-03	0.15212E-02	0.16109E-04	0.10590E-01
BENZO-01	0.15086E-04	0.59072E-04	0.29509E-06	0.49955E-02
BENZA-01	0.43326E-04	0.15256E-03	0.65925E-05	0.43212E-01
WATER	0.25940E-02	0.21887E-02	0.27302E-02	1.2475
OXYGEN	0.99141E-02	0.23050E-03	0.13170E-01	57.137
NITROGEN	0.43160	0.50162E-02	0.57505	114.64

BLOCK: E-302 MODEL: HEATER

INLET STREAM: 14
OUTLET STREAM: 16
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	3380.95	3380.95	0.00000
MASS(LB/HR)	190454.	190454.	0.00000
ENTHALPY(BTU/HR)	0.588878E+08	0.340602E+08	0.421609

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	F	110.000
PRESSURE DROP	PSI	5.00000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

```
                         ***  RESULTS  ***
  OUTLET TEMPERATURE     F                                  110.00
  OUTLET PRESSURE        PSIA                               159.74
  HEAT DUTY              BTU/HR                          -0.24828E+08
  OUTLET VAPOR FRACTION                                   0.45102


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)          X(I)          Y(I)          K(I)
     BENZENE         0.52796       0.93893       0.27732E-01   0.29536E-01
     PHENOL          0.27477E-01   0.50027E-01   0.27739E-04   0.55447E-03
     CATECHOL        0.39486E-03   0.71923E-03   0.27093E-07   0.37670E-04
     BENZO-01        0.15086E-04   0.27480E-04   0.38898E-09   0.14155E-04
     BENZA-01        0.43326E-04   0.78874E-04   0.56512E-07   0.71649E-03
     WATER           0.25940E-02   0.43427E-02   0.46542E-03   0.10717
     OXYGEN          0.99141E-02   0.38846E-03   0.21509E-01    55.369
     NITROGEN        0.43160       0.54895E-02   0.95027        173.11

BLOCK:  E-303    MODEL: HEATER
------------------------------
  INLET STREAM:          13
  OUTLET STREAM:         15
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            4021.24         4021.24         0.00000
      MASS(LB/HR    )            319238.         319238.         0.00000
      ENTHALPY(BTU/HR  )      0.838925E+08    0.569655E+08    0.320971

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

```
                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE                F                      285.000
  PRESSURE DROP                        PSI                      5.00000
  MAXIMUM NO. ITERATIONS                                       30
  CONVERGENCE TOLERANCE                                         0.000100000


                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                      285.00
  OUTLET PRESSURE       PSIA                                   164.74
  HEAT DUTY             BTU/HR                               -0.26927E+08
  OUTLET VAPOR FRACTION                                       0.30987E-01


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     BENZENE       0.81742       0.83151       0.37700       0.45339
     PHENOL        0.15132       0.15595       0.66902E-02   0.42900E-01
     CATECHOL      0.47133E-02   0.48625E-02   0.45760E-04   0.94108E-02
     BENZO-01      0.29621E-03   0.30564E-03   0.14077E-05   0.46058E-02
     BENZA-01      0.27247E-03   0.28081E-03   0.11721E-04   0.41740E-01
     WATER         0.20089E-02   0.19968E-02   0.23853E-02    1.1946
     OXYGEN        0.80237E-03   0.27986E-03   0.17142E-01    61.253
     NITROGEN      0.23162E-01   0.48210E-02   0.59672        123.78

BLOCK:  E-304    MODEL: HEATER
------------------------------
  INLET STREAM:          15
  OUTLET STREAM:         17
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
     MOLE(LBMOL/HR)            4021.24         4021.24         0.00000
     MASS(LB/HR    )           319238.         319238.         0.00000
     ENTHALPY(BTU/HR  )     0.569655E+08    0.319308E+08    0.439471
```

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

                        ***  INPUT DATA  ***
 TWO    PHASE  TP  FLASH
 SPECIFIED TEMPERATURE                F                      110.000
 PRESSURE DROP                        PSI                      5.00000
 MAXIMUM NO. ITERATIONS                                       30
 CONVERGENCE TOLERANCE                                         0.000100000



                         ***  RESULTS  ***
 OUTLET TEMPERATURE    F                                     110.00
 OUTLET PRESSURE       PSIA                                  159.74
 HEAT DUTY             BTU/HR                              -0.25035E+08
 OUTLET VAPOR FRACTION                                      0.19248E-01


 V-L PHASE EQUILIBRIUM :

    COMP            F(I)          X(I)          Y(I)          K(I)
    BENZENE        0.81742       0.83297       0.24974E-01   0.29982E-01
    PHENOL         0.15132       0.15429       0.74221E-04   0.48104E-03
    CATECHOL       0.47133E-02   0.48058E-02   0.13778E-06   0.28669E-04
    BENZO-01       0.29621E-03   0.30202E-03   0.36640E-08   0.12132E-04
    BENZA-01       0.27247E-03   0.27782E-03   0.19008E-06   0.68418E-03
    WATER          0.20089E-02   0.20445E-02   0.19100E-03   0.93418E-01
    OXYGEN         0.80237E-03   0.37015E-03   0.22825E-01    61.664
    NITROGEN       0.23162E-01   0.49342E-02   0.95193        192.92

BLOCK:  E-501    MODEL: HEATER
------------------------------
  INLET STREAM:          29
  OUTLET STREAM:         32
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE
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                  ***  MASS AND ENERGY BALANCE  ***
                                IN                OUT          RELATIVE DIFF.
 TOTAL BALANCE
    MOLE(LBMOL/HR)            672.000           672.000          0.00000
    MASS(LB/HR    )           63255.9           63255.9         0.115024E-15
    ENTHALPY(BTU/HR  )     -0.212700E+08     -0.378767E+08      0.438441

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

                      ***  INPUT DATA  ***
 TWO    PHASE  TP  FLASH
 SPECIFIED TEMPERATURE              F                      285.000
 PRESSURE DROP                      PSI                      5.00000
 MAXIMUM NO. ITERATIONS                                     30
 CONVERGENCE TOLERANCE                                       0.000100000


                       ***  RESULTS  ***
 OUTLET TEMPERATURE    F                                   285.00
 OUTLET PRESSURE       PSIA                                19.400
 HEAT DUTY             BTU/HR                          -0.16607E+08
 OUTLET VAPOR FRACTION                                      0.0000


 V-L PHASE EQUILIBRIUM :

    COMP            F(I)          X(I)          Y(I)          K(I)
    BENZENE      0.12656E-04   0.12656E-04   0.29910E-03    5.1304
    PHENOL       0.99849       0.99849       0.99734       0.21684
    CATECHOL     0.65060E-05   0.65060E-05   0.73805E-06   0.24627E-01
    BENZO-01     0.13997E-06   0.13997E-06   0.15119E-07   0.23450E-01
    BENZA-01     0.14917E-02   0.14917E-02   0.23575E-02   0.34310
    WATER        0.38529E-10   0.38529E-10   0.10263E-08    5.7828
```

```
BLOCK:  E-502    MODEL: HEATER
------------------------------
  INLET STREAM:          32
  OUTLET STREAM:         34
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           672.000          672.000          0.00000
      MASS(LB/HR    )         63255.9          63255.9          0.00000
      ENTHALPY(BTU/HR  )   -0.378767E+08    -0.429102E+08     0.117304

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

                         ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE              F                      113.000
  PRESSURE DROP                      PSI                      5.00000
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                       0.000100000



                          ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                   113.00
  OUTLET PRESSURE       PSIA                                14.400
  HEAT DUTY             BTU/HR                          -0.50335E+07
  OUTLET VAPOR FRACTION                                     0.0000


  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     BENZENE      0.12656E-04   0.12656E-04   0.24399E-02   0.62107
     PHENOL       0.99849       0.99849       0.99253       0.32024E-02
```

CATECHOL	0.65060E-05	0.65060E-05	0.14431E-06	0.71461E-04
BENZO-01	0.13997E-06	0.13997E-06	0.43529E-08	0.10019E-03
BENZA-01	0.14917E-02	0.14917E-02	0.50337E-02	0.10872E-01
WATER	0.38529E-10	0.38529E-10	0.48611E-08	0.40646

BLOCK: E-503 MODEL: HEATER

INLET STREAM: 31
OUTLET STREAM: 33
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	48.6759	48.6759	0.00000
MASS(LB/HR)	4890.76	4890.76	0.00000
ENTHALPY(BTU/HR)	-0.395293E+07	-0.424425E+07	0.686371E-01

*** CO2 EQUIVALENT SUMMARY ***

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

*** INPUT DATA ***

TWO PHASE TP FLASH		
SPECIFIED TEMPERATURE	F	285.000
PRESSURE DROP	PSI	5.00000
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

*** RESULTS ***

OUTLET TEMPERATURE	F	285.00
OUTLET PRESSURE	PSIA	15.000
HEAT DUTY	BTU/HR	-0.29131E+06
OUTLET VAPOR FRACTION		0.0000

```
  V-L PHASE EQUILIBRIUM :

     COMP            F(I)          X(I)          Y(I)          K(I)
     BENZENE       0.67150E-01   0.67150E-01   0.79469        8.9011
     PHENOL        0.48600       0.48600       0.18632       0.28834
     CATECHOL      0.41671       0.41671       0.14300E-01   0.25810E-01
     BENZO-01      0.25516E-01   0.25516E-01   0.11720E-02   0.34547E-01
     BENZA-01      0.46210E-02   0.46210E-02   0.35167E-02   0.57240
     WATER         0.53783E-06   0.53783E-06   0.46493E-05    6.5018

BLOCK:  E-504    MODEL: HEATER
------------------------------
  INLET STREAM:          33
  OUTLET STREAM:         35
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            48.6759         48.6759        0.00000
      MASS(LB/HR   )            4890.76         4890.76        0.00000
      ENTHALPY(BTU/HR  )     -0.424425E+07   -0.463684E+07   0.846693E-01

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

                        ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE              F                      113.000
  PRESSURE DROP                      PSI                      5.00000
  MAXIMUM NO. ITERATIONS                                     30
  CONVERGENCE TOLERANCE                                       0.000100000
```

```
                          ***  RESULTS  ***
  OUTLET TEMPERATURE     F                                  113.00
  OUTLET PRESSURE        PSIA                               10.000
  HEAT DUTY              BTU/HR                          -0.39260E+06
  OUTLET VAPOR FRACTION                                     0.0000


  V-L PHASE EQUILIBRIUM :

     COMP              F(I)           X(I)           Y(I)           K(I)
     BENZENE        0.67150E-01    0.67150E-01    0.97488         1.4383
     PHENOL         0.48600        0.48600        0.23624E-01    0.48158E-02
     CATECHOL       0.41671        0.41671        0.30273E-03    0.71972E-04
     BENZO-01       0.25516E-01    0.25516E-01    0.46713E-04    0.18137E-03
     BENZA-01       0.46210E-02    0.46210E-02    0.11433E-02    0.24511E-01
     WATER          0.53783E-06    0.53783E-06    0.24040E-05    0.44283

BLOCK:  MIX      MODEL: MIXER
------------------------------
  INLET STREAMS:          22          4
  OUTLET STREAM:          5
  PROPERTY OPTION SET:    PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            5813.70          5813.70          0.00000
      MASS(LB/HR    )           453120.          453120.         -0.256920E-15
      ENTHALPY(BTU/HR  )     0.139259E+09     0.139259E+09     -0.428012E-15

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

                          ***  INPUT DATA  ***
```

```
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  P-101    MODEL: PUMP
------------------------------
  INLET STREAM:          3
  OUTLET STREAM:         4
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            840.000          840.000          0.00000
      MASS(LB/HR   )            65615.5          65615.5          0.00000
      ENTHALPY(BTU/HR  )      0.183251E+08     0.185690E+08    -0.131336E-01

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

                        ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                  652.862
   DRIVER EFFICIENCY                                        1.00000

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

                         ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                        1,212.20
   PRESSURE CHANGE  PSI                                   638.162
   NPSH AVAILABLE   FT-LBF/LB                              32.6969
   FLUID POWER  HP                                         56.2602
   BRAKE POWER  HP                                         95.8473
   ELECTRICITY  KW                                         71.4733
```

```
   PUMP EFFICIENCY USED                                    0.58698
   NET WORK REQUIRED  HP                                  95.8473
   HEAD DEVELOPED FT-LBF/LB                            1,697.70

BLOCK:  P-102    MODEL: PUMP
------------------------------
  INLET STREAM:          21
  OUTLET STREAM:         22
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            4973.70          4973.70          0.00000
      MASS(LB/HR    )           387504.          387504.         0.300423E-15
      ENTHALPY(BTU/HR  )     0.119530E+09     0.120690E+09    -0.961765E-02

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

                        ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                 652.862
   DRIVER EFFICIENCY                                       1.00000

   FLASH SPECIFICATIONS:
   2 PHASE FLASH
   MAXIMUM NUMBER OF ITERATIONS                           100
   TOLERANCE                                               0.000100000

                         ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                       7,596.88
   PRESSURE CHANGE  PSI                                  632.862
   NPSH AVAILABLE   FT-LBF/LB                              0.0
   FLUID POWER  HP                                       349.657
   BRAKE POWER  HP                                       456.195
   ELECTRICITY  KW                                       340.185
   PUMP EFFICIENCY USED                                    0.76646
   NET WORK REQUIRED  HP                                 456.195
```

```
   HEAD DEVELOPED FT-LBF/LB                              1,786.61

BLOCK:  P-301    MODEL: PUMP
------------------------------
  INLET STREAM:          11
  OUTLET STREAM:         13
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            4021.24          4021.24          0.00000
      MASS(LB/HR    )            319238.          319238.       -0.364666E-15
      ENTHALPY(BTU/HR  )       0.842611E+08     0.838925E+08     0.437440E-02

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

                         ***  INPUT DATA  ***
   EQUIPMENT TYPE: TURBINE
   OUTLET PRESSURE  PSIA                                  169.736
   PUMP EFFICIENCY                                          0.60000
   DRIVER EFFICIENCY                                        1.00000

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

                         ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                         7,892.31
   PRESSURE CHANGE  PSI                                   -420.632
   NPSH AVAILABLE   FT-LBF/LB                               0.0
   FLUID POWER  HP                                        -241.437
   BRAKE POWER  HP                                        -144.862
   ELECTRICITY  KW                                        -108.024
   PUMP EFFICIENCY USED                                     0.60000
```

```
   NET WORK REQUIRED  HP                                  -144.862
   HEAD DEVELOPED FT-LBF/LB                            -1,497.45

BLOCK:  P-403    MODEL: PUMP
------------------------------
  INLET STREAM:          25
  OUTLET STREAM:         26
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)           695.970          695.970          0.00000
      MASS(LB/HR    )          65462.2          65462.2        -0.444590E-15
      ENTHALPY(BTU/HR  )    -0.358110E+08    -0.358074E+08    -0.101587E-03

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

                       ***  INPUT DATA  ***
   OUTLET PRESSURE  PSIA                                  30.0000
   DRIVER EFFICIENCY                                       1.00000

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

                       ***  RESULTS  ***
   VOLUMETRIC FLOW RATE  CUFT/HR                       1,139.24
   PRESSURE CHANGE  PSI                                   10.00000
   NPSH AVAILABLE   FT-LBF/LB                              0.0
   FLUID POWER  HP                                         0.82854
   BRAKE POWER  HP                                         1.42976
   ELECTRICITY  KW                                         1.06617
   PUMP EFFICIENCY USED                                    0.57950
   NET WORK REQUIRED  HP                                   1.42976
```

```
   HEAD DEVELOPED FT-LBF/LB                                25.0603

BLOCK:  PRODMIX  MODEL: MIXER
------------------------------
  INLET STREAMS:          30          27          28
  OUTLET STREAM:          31
  PROPERTY OPTION SET:    PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            48.6759          48.6759          0.00000
      MASS(LB/HR    )            4890.76          4890.76       -0.185962E-15
      ENTHALPY(BTU/HR  )      -0.395293E+07    -0.395293E+07      0.00000

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

                         ***  INPUT DATA  ***
  TWO    PHASE      FLASH
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000
  OUTLET PRESSURE:  MINIMUM OF INLET STREAM PRESSURES

BLOCK:  R-201-4  MODEL: RSTOIC
------------------------------
  INLET STREAM:           8
  OUTLET STREAM:          9
  PROPERTY OPTION SET:    PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                             IN           OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(LBMOL/HR)          7774.83       7402.19       -372.641     -0.267271E-06
  MASS(LB/HR    )         509692.       509692.                    -0.166542E-06
  ENTHALPY(BTU/HR  )    0.309315E+09  0.250539E+09                  0.190018

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

```
 FEED STREAMS CO2E             0.00000      LB/HR
 PRODUCT STREAMS CO2E          0.00000      LB/HR
 NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
 UTILITIES CO2E PRODUCTION     0.00000      LB/HR
 TOTAL CO2E PRODUCTION         0.00000      LB/HR

                       ***  INPUT DATA  ***
STOICHIOMETRY MATRIX:

 REACTION #   1:
  SUBSTREAM MIXED   :
  BENZENE   -1.00    PHENOL     1.00    OXYGEN   -0.500

 REACTION #   2:
  SUBSTREAM MIXED   :
  BENZENE   -7.00    BENZO-01   6.00    WATER     3.00    OXYGEN    -7.50

 REACTION #   3:
  SUBSTREAM MIXED   :
  BENZENE   -7.00    BENZA-01   6.00    WATER     3.00    OXYGEN    -4.50

 REACTION #   4:
  SUBSTREAM MIXED   :
  BENZENE   -1.00    CATECHOL   1.00    OXYGEN    -1.00


REACTION CONVERSION SPECS: NUMBER=    4
  REACTION #   1:
  SUBSTREAM:MIXED    KEY COMP:BENZENE  CONV FRAC: 0.1210
  REACTION #   2:
  SUBSTREAM:MIXED    KEY COMP:BENZENE  CONV FRAC: 0.2500E-03
  REACTION #   3:
  SUBSTREAM:MIXED    KEY COMP:BENZENE  CONV FRAC: 0.2500E-03
  REACTION #   4:
  SUBSTREAM:MIXED    KEY COMP:BENZENE  CONV FRAC: 0.3500E-02



TWO    PHASE  TP  FLASH
SPECIFIED TEMPERATURE F                          662.000
SPECIFIED PRESSURE    PSIA                       594.847
```

MAXIMUM NO. ITERATIONS	100
CONVERGENCE TOLERANCE	0.000100000
SIMULTANEOUS REACTIONS	
GENERATE COMBUSTION REACTIONS FOR FEED SPECIES	NO

*** RESULTS ***

OUTLET TEMPERATURE	F	662.00
OUTLET PRESSURE	PSIA	594.85
HEAT DUTY	BTU/HR	-0.58775E+08
VAPOR FRACTION		1.0000

HEAT OF REACTIONS:

REACTION NUMBER	REFERENCE COMPONENT	HEAT OF REACTION BTU/LBMOL
1	BENZENE	-77188.
2	BENZENE	-0.18879E+06
3	BENZENE	-93858.
4	BENZENE	-0.15275E+06

REACTION EXTENTS:

REACTION NUMBER	REACTION EXTENT LBMOL/HR
1	701.39
2	0.20702
3	0.20702
4	20.288

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
BENZENE	0.68521	0.75494	0.68521	1.5569
PHENOL	0.94756E-01	0.13245	0.94756E-01	1.2272
CATECHOL	0.27408E-02	0.43111E-02	0.27408E-02	1.0906
BENZO-01	0.16781E-03	0.32143E-03	0.16781E-03	0.89554
BENZA-01	0.16781E-03	0.25909E-03	0.16781E-03	1.1110
WATER	0.22759E-02	0.19196E-02	0.22759E-02	2.0338

```
     OXYGEN            0.49641E-02    0.26428E-02    0.49641E-02     3.2221
     NITROGEN          0.20972        0.10315        0.20972         3.4874

BLOCK:  T-301    MODEL: FLASH2
------------------------------
  INLET STREAMS:          17          16
  OUTLET VAPOR STREAM:    18
  OUTLET LIQUID STREAM:   19
  PROPERTY OPTION SET:    PENG-ROB  STANDARD PR EQUATION OF STATE

                    ***  MASS AND ENERGY BALANCE  ***
                                 IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            7402.19          7402.19          0.00000
      MASS(LB/HR    )           509692.          509692.          0.00000
      ENTHALPY(BTU/HR  )      0.659909E+08     0.659909E+08    -0.204943E-08

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

                       ***  INPUT DATA  ***
  TWO    PHASE  PQ  FLASH
  PRESSURE DROP         PSI                                  0.0
  SPECIFIED HEAT DUTY   BTU/HR                               0.0
  MAXIMUM NO. ITERATIONS                                    30
  CONVERGENCE TOLERANCE                                      0.000100000

                       ***  RESULTS  ***
  OUTLET TEMPERATURE    F                                    110.12
  OUTLET PRESSURE       PSIA                                 159.74
  VAPOR FRACTION                                            0.21606


  V-L PHASE EQUILIBRIUM :

     COMP             F(I)          X(I)          Y(I)          K(I)
     BENZENE          0.68521       0.86692       0.25883E-01   0.29856E-01
```

PHENOL	0.94756E-01	0.12085	0.60960E-04	0.50441E-03
CATECHOL	0.27408E-02	0.34962E-02	0.10973E-06	0.31386E-04
BENZO-01	0.16781E-03	0.21405E-03	0.27341E-08	0.12773E-04
BENZA-01	0.16781E-03	0.21402E-03	0.14876E-06	0.69507E-03
WATER	0.22761E-02	0.28272E-02	0.27651E-03	0.97805E-01
OXYGEN	0.49641E-02	0.36351E-03	0.21657E-01	59.579
NITROGEN	0.20972	0.51106E-02	0.95212	186.31

BLOCK: T-302 MODEL: RADFRAC

INLETS - 19 STAGE 6
OUTLETS - 20 STAGE 1
21 STAGE 1
23 STAGE 12
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	5802.91	5802.91	0.406005E-06
MASS(LB/HR)	462677.	462676.	0.209304E-06
ENTHALPY(BTU/HR)	0.642416E+08	0.833964E+08	-0.229683

*** CO2 EQUIVALENT SUMMARY ***

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

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

**** INPUT PARAMETERS ****

NUMBER OF STAGES	12
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD

```
 HYDRAULIC PARAMETER CALCULATIONS                          NO
 INSIDE LOOP CONVERGENCE METHOD                            BROYDEN
 DESIGN SPECIFICATION METHOD                               NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                     200
 MAXIMUM NO. OF INSIDE LOOP ITERATIONS                       10
 MAXIMUM NUMBER OF FLASH ITERATIONS                          30
 FLASH TOLERANCE                                            0.000100000
 OUTSIDE LOOP CONVERGENCE TOLERANCE                         0.000100000

****    COL-SPECS    ****

 MOLAR VAPOR DIST / TOTAL DIST                              0.020000
 MOLAR REFLUX RATIO                                         0.50000
 MOLAR BOTTOMS RATE              LBMOL/HR                  740.000

****     PROFILES    ****

 P-SPEC          STAGE   1  PRES, PSIA                      20.0000

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


***    COMPONENT SPLIT FRACTIONS    ***

                         OUTLET STREAMS
                         --------------
               20            21            23
 COMPONENT:
 BENZENE      .13992E-01    .98528        .72327E-03
 PHENOL       .85907E-08    .15160E-04    .99998
 CATECHOL     .78239E-13    .11426E-08    1.0000
 BENZO-01     0.0000        .11379E-10    1.0000
 BENZA-01     .95209E-08    .15912E-04    .99998
 WATER        .48746E-01    .95125        .18363E-05
 OXYGEN       .89838        .10162        0.0000
 NITROGEN     .95836        .41638E-01    0.0000


***     SUMMARY OF KEY RESULTS     ***
```

TOP STAGE TEMPERATURE	F	172.408
BOTTOM STAGE TEMPERATURE	F	389.798
TOP STAGE LIQUID FLOW	LBMOL/HR	2,537.60
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	727.706
TOP STAGE VAPOR FLOW	LBMOL/HR	101.504
BOILUP VAPOR FLOW	LBMOL/HR	5,956.98
MOLAR REFLUX RATIO		0.50000
MOLAR BOILUP RATIO		8.18597
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.103386+09
REBOILER DUTY	BTU/HR	0.122541+09

**** MANIPULATED VARIABLES ****

		BOUNDS		CALCULATED
		LOWER	UPPER	VALUE
MOLAR BOTTOMS RATE	LBMOL/HR	500.00	1000.0	727.71

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MOLE-FRAC	STREAMS: 23 COMPS: BENZENE		0.50000E-02	0.50000E-02

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

DEW POINT	0.12348E-05	STAGE= 10	
BUBBLE POINT	0.32994E-05	STAGE= 10	
COMPONENT MASS BALANCE	0.20126E-05	STAGE= 1	COMP=NITROGEN
ENERGY BALANCE	0.16773E-05	STAGE= 11	

**** PROFILES ****

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

STAGE	TEMPERATURE	PRESSURE	ENTHALPY BTU/LBMOL		HEAT DUTY
	F	PSIA	LIQUID	VAPOR	BTU/HR

1	172.41	20.000	24032.	25454.	-.10339+09
2	200.83	22.000	25298.	37632.	
4	201.82	22.280	25210.	37774.	
5	202.90	22.420	24361.	37757.	
6	207.75	22.560	18857.	37735.	
7	208.30	22.700	18917.	37994.	
8	209.07	22.840	18518.	38060.	
11	360.98	23.260	-49361.	-4022.9	
12	389.80	23.400	-53204.	-28320.	.12254+09

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	7511.	101.5				4973.6980	101.5040
2	2719.	7613.					
4	2699.	7789.					
5	2620.	7775.		33.3296			
6	9871.	7662.	5769.5807				
7	9871.	9144.					
8	9764.	9143.					
11	6685.	5730.					
12	727.7	5957.				727.7058	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5852E+06	6369.				.38750+06	6369.4908
2	0.2122E+06	0.5916E+06					
4	0.2108E+06	0.6058E+06					
5	0.2051E+06	0.6047E+06		1219.9642			
6	0.7833E+06	0.5977E+06	.46146+06				
7	0.7835E+06	0.7145E+06					
8	0.7760E+06	0.7147E+06					
11	0.6252E+06	0.5044E+06					
12	0.6880E+05	0.5564E+06				.68803+05	

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.99657	0.21376E-05	0.46608E-11	0.28418E-14	0.39731E-08
2	0.99902	0.39880E-04	0.58438E-09	0.91090E-12	0.73985E-07

4	0.99741	0.18976E-02	0.11362E-05	0.11433E-07	0.35129E-05
5	0.98698	0.12256E-01	0.49089E-04	0.12487E-05	0.22563E-04
6	0.92201	0.74969E-01	0.20709E-02	0.12623E-03	0.13305E-03
7	0.92217	0.75277E-01	0.20714E-02	0.12625E-03	0.13404E-03
8	0.91706	0.80499E-01	0.20964E-02	0.12772E-03	0.15083E-03
11	0.46966E-01	0.94253	0.80681E-02	0.44353E-03	0.19920E-02
12	0.50000E-02	0.96371	0.27879E-01	0.17069E-02	0.17066E-02

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

STAGE	WATER	OXYGEN	NITROGEN
1	0.31377E-02	0.43099E-04	0.24827E-03
2	0.93422E-03	0.74574E-06	0.42142E-05
4	0.68722E-03	0.70130E-06	0.40897E-05
5	0.68656E-03	0.69981E-06	0.40893E-05
6	0.69159E-03	0.19738E-06	0.46370E-06
7	0.21777E-03	0.52090E-09	0.51343E-09
8	0.68578E-04	0.13763E-11	0.57009E-12
11	0.52207E-06	0.71554E-20	0.30355E-21
12	0.41398E-07	0.94950E-23	0.21905E-24

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.69345	0.59354E-07	0.15638E-13	0.35870E-17	0.11649E-09
2	0.99253	0.21099E-05	0.45988E-11	0.28039E-14	0.39217E-08
4	0.99347	0.10142E-03	0.90808E-08	0.35834E-10	0.18798E-06
5	0.99290	0.66026E-03	0.39451E-06	0.39698E-08	0.12223E-05
6	0.99288	0.41906E-02	0.16783E-04	0.42691E-06	0.77139E-05
7	0.99499	0.42386E-02	0.16975E-04	0.43201E-06	0.78201E-05
8	0.99517	0.45657E-02	0.17316E-04	0.44255E-06	0.88790E-05
11	0.38239	0.61495	0.97667E-03	0.44215E-04	0.16336E-02
12	0.52093E-01	0.93994	0.56479E-02	0.28920E-03	0.20269E-02

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

STAGE	WATER	OXYGEN	NITROGEN
1	0.78788E-02	0.18669E-01	0.28000
2	0.32010E-02	0.29145E-03	0.39783E-02
4	0.23533E-02	0.27104E-03	0.38086E-02
5	0.23488E-02	0.27156E-03	0.38159E-02
6	0.23680E-02	0.81264E-04	0.45566E-03
7	0.74663E-03	0.21309E-06	0.50060E-06
8	0.23510E-03	0.56236E-09	0.55429E-09
11	0.58205E-05	0.59997E-17	0.48324E-18

12	0.58078E-06	0.80283E-20	0.34060E-21

**** K-VALUES ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.69584	0.27767E-01	0.33552E-02	0.12622E-02	0.29320E-01
2	0.99350	0.52906E-01	0.78696E-02	0.30782E-02	0.53006E-01
4	0.99605	0.53446E-01	0.79922E-02	0.31342E-02	0.53512E-01
5	1.0060	0.53873E-01	0.80366E-02	0.31792E-02	0.54172E-01
6	1.0769	0.55898E-01	0.81040E-02	0.33820E-02	0.57977E-01
7	1.0790	0.56307E-01	0.81949E-02	0.34218E-02	0.58342E-01
8	1.0852	0.56718E-01	0.82596E-02	0.34650E-02	0.58866E-01
11	8.1417	0.65245	0.12105	0.99688E-01	0.82006
12	10.419	0.97534	0.20258	0.16943	1.1877

**** K-VALUES ****

STAGE	WATER	OXYGEN	NITROGEN
1	2.5110	433.18	1127.8
2	3.4263	390.82	944.02
4	3.4244	386.49	931.28
5	3.4211	388.05	933.13
6	3.4240	411.71	982.66
7	3.4285	409.08	975.02
8	3.4283	408.59	972.29
11	11.149	838.49	1592.0
12	14.029	845.53	1554.9

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.99916	0.25821E-05	0.65872E-11	0.44544E-14	0.54118E-08
2	0.99973	0.48082E-04	0.82436E-09	0.14251E-11	0.10059E-06
4	0.99755	0.22866E-02	0.16019E-05	0.17877E-07	0.47732E-05
5	0.98500	0.14737E-01	0.69059E-04	0.19483E-05	0.30592E-04
6	0.90768	0.88920E-01	0.28739E-02	0.19428E-03	0.17795E-03
7	0.90746	0.89248E-01	0.28734E-02	0.19423E-03	0.17920E-03
8	0.90136	0.95326E-01	0.29046E-02	0.19626E-03	0.20141E-03
11	0.39226E-01	0.94844	0.94988E-02	0.57914E-03	0.22603E-02
12	0.41309E-02	0.95928	0.32469E-01	0.22048E-02	0.19156E-02

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

STAGE	WATER	OXYGEN	NITROGEN
1	0.72554E-03	0.17701E-04	0.89269E-04
2	0.21561E-03	0.30571E-06	0.15124E-05

4	0.15852E-03	0.28732E-06	0.14669E-05
5	0.15802E-03	0.28610E-06	0.14636E-05
6	0.15702E-03	0.79599E-07	0.16371E-06
7	0.49423E-04	0.20998E-09	0.18119E-09
8	0.15545E-04	0.55416E-12	0.20095E-12
11	0.10056E-06	0.24481E-20	0.90920E-22
12	0.78881E-08	0.32135E-23	0.64902E-25

**** MASS-Y-PROFILE ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.86322	0.89019E-07	0.27441E-13	0.69808E-17	0.19701E-09
2	0.99770	0.25552E-05	0.65165E-11	0.44065E-14	0.53557E-08
4	0.99785	0.12273E-03	0.12857E-07	0.56270E-10	0.25652E-06
5	0.99717	0.79891E-03	0.55851E-06	0.62331E-08	0.16677E-05
6	0.99417	0.50555E-02	0.23689E-04	0.66829E-06	0.10494E-04
7	0.99469	0.51053E-02	0.23921E-04	0.67520E-06	0.10621E-04
8	0.99441	0.54966E-02	0.24390E-04	0.69135E-06	0.12054E-04
11	0.33931	0.65744	0.12217E-02	0.61338E-04	0.19693E-02
12	0.43566E-01	0.94709	0.66583E-02	0.37812E-03	0.23030E-02

**** MASS-Y-PROFILE ****

STAGE	WATER	OXYGEN	NITROGEN
1	0.22619E-02	0.95202E-02	0.12500
2	0.74208E-03	0.12001E-03	0.14342E-02
4	0.54515E-03	0.11152E-03	0.13719E-02
5	0.54403E-03	0.11172E-03	0.13743E-02
6	0.54684E-03	0.33332E-04	0.16362E-03
7	0.17214E-03	0.87264E-07	0.17947E-06
8	0.54180E-04	0.23019E-09	0.19863E-09
11	0.11911E-05	0.21809E-17	0.15378E-18
12	0.11202E-06	0.27504E-20	0.10215E-21

****
***** HYDRAULIC PARAMETERS *****
****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

	TEMPERATURE F	
STAGE	LIQUID FROM	VAPOR TO
1	172.41	200.83
2	200.83	201.31
4	201.82	202.90
5	202.90	207.54
6	207.75	208.30
7	208.30	209.07
8	209.07	214.63
11	360.98	389.80
12	389.80	389.80

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	0.58521E+06	0.59158E+06	11473.	0.23555E+07	77.911	77.709
2	0.21220E+06	0.60608E+06	4252.8	0.23974E+07	78.058	77.765
4	0.21084E+06	0.60471E+06	4226.6	0.23667E+07	78.103	77.779
5	0.20506E+06	0.59894E+06	4102.4	0.23606E+07	78.270	77.833
6	0.78327E+06	0.71447E+06	15443.	0.27713E+07	79.347	78.137
7	0.78354E+06	0.71474E+06	15455.	0.27569E+07	79.381	78.173
8	0.77599E+06	0.70718E+06	15293.	0.27321E+07	79.474	78.261
11	0.62520E+06	0.55640E+06	10871.	0.22435E+07	93.527	93.402
12	68803.	0.0000	1201.4	0.0000	94.547	

STAGE	DENSITY LB/CUFT LIQUID FROM	DENSITY LB/CUFT VAPOR TO	VISCOSITY CP LIQUID FROM	VISCOSITY CP VAPOR TO	SURFACE TENSION DYNE/CM LIQUID FROM
1	51.008	0.25115	0.32675	0.94177E-02	16.884
2	49.898	0.25280	0.27900	0.94213E-02	14.717
4	49.883	0.25551	0.27819	0.94439E-02	14.661
5	49.985	0.25372	0.28048	0.95064E-02	14.691
6	50.720	0.25781	0.29801	0.94892E-02	15.099
7	50.700	0.25926	0.29715	0.94987E-02	19.291
8	50.741	0.25884	0.29780	0.95726E-02	19.280
11	57.510	0.24801	0.18720	0.11441E-01	21.868
12	57.268		0.15388		20.561

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.69413E-01	0.16569E+06	0.11805E+07
2	-2.1674	0.24922E-01	0.17108E+06	0.12054E+07
4	-.22055E-01	0.24953E-01	0.16982E+06	0.11963E+07
5	0.29651E-01	0.24393E-01	0.16861E+06	0.11890E+07
6	-5.3926	0.78160E-01	0.19809E+06	0.14071E+07
7	4.1915	0.78393E-01	0.19765E+06	0.14037E+07
8	-.10626E-01	0.78371E-01	0.19564E+06	0.13900E+07
11	-2.0613	0.73790E-01	0.14765E+06	0.11173E+07
12	-1.3075		0.0000	0.0000

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER	2
ENDING STAGE NUMBER	5
FLOODING CALCULATION METHOD	GLITSCH6

DESIGN PARAMETERS

PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		4
TRAY SPACING	FT	1.50000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		2
COLUMN DIAMETER	FT	15.4790
DC AREA/COLUMN AREA		0.093750
SIDE DOWNCOMER VELOCITY	FT/SEC	0.066961
FLOW PATH LENGTH	FT	2.90471
SIDE DOWNCOMER WIDTH	FT	0.94159
SIDE WEIR LENGTH	FT	7.39952
CENTER DOWNCOMER WIDTH	FT	0.60801
CENTER WEIR LENGTH	FT	15.4670
OFF-CENTER DOWNCOMER WIDTH	FT	0.68447
OFF-CENTER SHORT WEIR LENGTH	FT	13.3780
OFF-CENTER LONG WEIR LENGTH	FT	14.0860
TRAY CENTER TO OCDC CENTER	FT	3.55095

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
2	15.479	188.18	37.636	4.4105
3	15.479	188.18	37.636	4.4105
4	15.479	188.18	37.636	4.4105
5	15.479	188.18	37.636	4.4105

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
2	0.8000	0.1202	0.6391	0.3933
3	0.7975	0.1196	0.6366	0.3917
4	0.7942	0.1188	0.6330	0.3895
5	0.7880	0.1177	0.6261	0.3853

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.1159	0.6076	0.1786	0.5487
3	0.1157	0.6076	0.1789	0.5473
4	0.1152	0.6076	0.1792	0.5453
5	0.1127	0.6076	0.1797	0.5412

****
*** SECTION 2 ***
****

STARTING STAGE NUMBER		6
ENDING STAGE NUMBER		11
FLOODING CALCULATION METHOD		GLITSCH6
DESIGN PARAMETERS		
PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000
TRAY SPECIFICATIONS		
TRAY TYPE		SIEVE

NUMBER OF PASSES		4
TRAY SPACING	FT	1.50000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		7
COLUMN DIAMETER	FT	17.2331
DC AREA/COLUMN AREA		0.093750
SIDE DOWNCOMER VELOCITY	FT/SEC	0.19632
FLOW PATH LENGTH	FT	3.23388
SIDE DOWNCOMER WIDTH	FT	1.04829
SIDE WEIR LENGTH	FT	8.23806
CENTER DOWNCOMER WIDTH	FT	0.67692
CENTER WEIR LENGTH	FT	17.2198
OFF-CENTER DOWNCOMER WIDTH	FT	0.76204
OFF-CENTER SHORT WEIR LENGTH	FT	14.8940
OFF-CENTER LONG WEIR LENGTH	FT	15.6822
TRAY CENTER TO OCDC CENTER	FT	3.95335

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
6	17.233	233.25	46.649	5.4667
7	17.233	233.25	46.649	5.4667
8	17.233	233.25	46.649	5.4667
9	17.233	233.25	46.649	5.4667
10	17.233	233.25	46.649	5.4667
11	17.233	233.25	46.649	5.4667

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
6	0.8015	0.1179	0.7220	0.4443
7	0.8000	0.1182	0.7237	0.4454
8	0.7918	0.1166	0.7150	0.4400

```
  9    0.7203      0.1048      0.6416      0.3948
 10    0.5508      0.8538E-01  0.5052      0.3109
 11    0.5941      0.9299E-01  0.5328      0.3279

      HEIGHT      DC REL      TR LIQ REL  FRA APPR TO
STAGE OVER WEIR   FROTH DENS  FROTH DENS  SYS LIMIT
       FT
  6    0.2509      0.6077      0.1835      0.5133
  7    0.2508      0.6077      0.1837      0.4816
  8    0.2483      0.6077      0.1846      0.4768
  9    0.2230      0.6078      0.1927      0.4280
 10    0.1670      0.6082      0.2204      0.3232
 11    0.1819      0.6082      0.2088      0.3579

BLOCK:  T-401    MODEL: RADFRAC
------------------------------
   INLETS    - 23        STAGE   6
   OUTLETS   - 24        STAGE   1
               25        STAGE   1
               27        STAGE  12
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                    IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            727.706         727.706          0.00000
      MASS(LB/HR   )            68802.7         68802.7       -0.897403E-12
      ENTHALPY(BTU/HR  )      -0.387169E+08   -0.389208E+08    0.523860E-02

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


                          **********************
                          ****  INPUT DATA  ****
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****    INPUT PARAMETERS    ****

 NUMBER OF STAGES                                          12
 ALGORITHM OPTION                                      STANDARD
 ABSORBER OPTION                                       NO
 INITIALIZATION OPTION                                 STANDARD
 HYDRAULIC PARAMETER CALCULATIONS                      NO
 INSIDE LOOP CONVERGENCE METHOD                        BROYDEN
 DESIGN SPECIFICATION METHOD                           NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
 MAXIMUM NO. OF INSIDE LOOP ITERATIONS                 10
 MAXIMUM NUMBER OF FLASH ITERATIONS                    30
 FLASH TOLERANCE                                        0.000100000
 OUTSIDE LOOP CONVERGENCE TOLERANCE                     0.000100000

****    COL-SPECS    ****

 MOLAR VAPOR DIST / TOTAL DIST                          0.0100000
 MOLAR REFLUX RATIO                                     4.00000
 MOLAR DISTILLATE RATE          LBMOL/HR               703.000

****     PROFILES    ****

 P-SPEC          STAGE    1  PRES, PSIA                 20.0000

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


***    COMPONENT SPLIT FRACTIONS    ***

                          OUTLET STREAMS
                          --------------
               24             25             27
 COMPONENT:
 BENZENE      .99337E-01     .90066         .70054E-10
 PHENOL       .94881E-02     .98598         .45342E-02
 CATECHOL     .43768E-06     .23042E-03     .99977
 BENZO-01     .13445E-06     .85198E-04     .99991
 BENZA-01     .11738E-01     .98773         .53643E-03
 WATER        .13014         .86986         .25440E-10
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  ***     SUMMARY OF KEY RESULTS     ***

   TOP STAGE TEMPERATURE           F                      377.141
   BOTTOM STAGE TEMPERATURE        F                      476.105
   TOP STAGE LIQUID FLOW           LBMOL/HR             2,812.00
   BOTTOM STAGE LIQUID FLOW        LBMOL/HR               24.7059
   TOP STAGE VAPOR FLOW            LBMOL/HR                7.03000
   BOILUP VAPOR FLOW               LBMOL/HR             2,818.22
   MOLAR REFLUX RATIO                                      4.00000
   MOLAR BOILUP RATIO                                    114.071
   CONDENSER DUTY (W/O SUBCOOL)    BTU/HR                 -0.697989+08
   REBOILER DUTY                   BTU/HR                  0.695950+08

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

   DEW POINT                       0.13662E-05  STAGE= 12
   BUBBLE POINT                    0.40973E-06  STAGE= 11
   COMPONENT MASS BALANCE          0.13523E-05  STAGE=  6 COMP=BENZO-01
   ENERGY BALANCE                  0.78148E-06  STAGE= 12


  ****     PROFILES    ****

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

                                          ENTHALPY
STAGE  TEMPERATURE   PRESSURE             BTU/LBMOL          HEAT DUTY
       F             PSIA           LIQUID       VAPOR        BTU/HR

   1   377.14        20.000       -51455.      -28365.      -.69799+08
   2   386.93        22.000       -51329.      -31551.
   3   387.65        22.150       -51333.      -31792.
   4   388.17        22.300       -51345.      -31804.
   5   388.74        22.450       -51446.      -31813.
   6   389.56        22.600       -51896.      -31878.
   7   390.22        22.750       -52046.      -31969.
  11   437.24        23.350       -97680.      -47391.
  12   476.10        23.500     -0.11780E+06   -72809.       .69595+08
```

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	3508.	7.030				695.9700	7.0300
2	2874.	3515.					
3	2875.	3577.					
4	2875.	3578.					
5	2872.	3578.					
6	3599.	3575.	723.1351	4.5707			
7	3595.	3574.					
11	2843.	3154.					
12	24.71	2818.				24.7058	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.3300E+06	656.0				.65462+05	656.0067
2	0.2705E+06	0.3306E+06					
3	0.2706E+06	0.3366E+06					
4	0.2706E+06	0.3367E+06					
5	0.2704E+06	0.3367E+06					
6	0.3392E+06	0.3365E+06	.68376+05	427.0717			
7	0.3390E+06	0.3365E+06					
11	0.2962E+06	0.3093E+06					
12	2684.	0.2935E+06				2684.4654	

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.47087E-02	0.99352	0.67168E-05	0.15206E-06	0.17625E-02
2	0.44876E-03	0.99806	0.32541E-04	0.89223E-06	0.14609E-02
3	0.12892E-03	0.99848	0.13236E-03	0.43602E-05	0.12576E-02
4	0.10512E-03	0.99823	0.51749E-03	0.20579E-04	0.11227E-02
5	0.10350E-03	0.99677	0.19983E-02	0.96106E-04	0.10322E-02
6	0.10317E-03	0.99084	0.76506E-02	0.44407E-03	0.96680E-03
7	0.97414E-05	0.98901	0.96127E-02	0.56961E-03	0.79807E-03
11	0.31116E-09	0.40281	0.55294	0.44131E-01	0.12211E-03
12	0.10317E-10	0.12871	0.82099	0.50272E-01	0.26965E-04

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

STAGE	WATER

1	0.37653E-07
2	0.26424E-08
3	0.72081E-09
4	0.61655E-09
5	0.61223E-09
6	0.61313E-09
7	0.42509E-10
11	0.72175E-15
12	0.31021E-16

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.51414E-01	0.94651	0.12631E-05	0.23757E-07	0.20735E-02
2	0.48021E-02	0.99343	0.67059E-05	0.15180E-06	0.17631E-02
3	0.13779E-02	0.99707	0.27454E-04	0.74649E-06	0.15208E-02
4	0.11205E-02	0.99741	0.10766E-03	0.35331E-05	0.13574E-02
5	0.11014E-02	0.99722	0.41712E-03	0.16565E-04	0.12490E-02
6	0.11009E-02	0.99604	0.16066E-02	0.77237E-04	0.11765E-02
7	0.10389E-03	0.99679	0.20284E-02	0.99635E-04	0.97330E-03
11	0.63016E-08	0.76786	0.21241	0.19405E-01	0.32537E-03
12	0.31380E-09	0.40521	0.55059	0.44077E-01	0.12294E-03

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

STAGE	WATER
1	0.55769E-06
2	0.38693E-07
3	0.10546E-07
4	0.89989E-08
5	0.89156E-08
6	0.89186E-08
7	0.61737E-09
11	0.13294E-13
12	0.72780E-15

**** K-VALUES ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	10.919	0.95268	0.18805	0.15624	1.1765
2	10.701	0.99536	0.20607	0.17013	1.2069
3	10.688	0.99859	0.20743	0.17121	1.2093
4	10.660	0.99918	0.20804	0.17169	1.2090
5	10.642	1.0004	0.20874	0.17236	1.2100
6	10.670	1.0053	0.21000	0.17393	1.2169

7	10.665	1.0079	0.21101	0.17492	1.2196
11	20.252	1.9063	0.38414	0.43970	2.6646
12	30.415	3.1483	0.67064	0.87677	4.5593

**** K-VALUES ****

STAGE	WATER
1	14.811
2	14.643
3	14.631
4	14.595
5	14.563
6	14.546
7	14.523
11	18.419
12	23.462

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.39104E-02	0.99409	0.78632E-05	0.19743E-06	0.19886E-02
2	0.37243E-03	0.99794	0.38069E-04	0.11577E-05	0.16472E-02
3	0.10699E-03	0.99831	0.15483E-03	0.56570E-05	0.14178E-02
4	0.87228E-04	0.99802	0.60533E-03	0.26697E-04	0.12657E-02
5	0.85863E-04	0.99629	0.23368E-02	0.12465E-03	0.11634E-02
6	0.85503E-04	0.98931	0.89375E-02	0.57535E-03	0.10885E-02
7	0.80699E-05	0.98713	0.11225E-01	0.73774E-03	0.89821E-03
11	0.23327E-09	0.36382	0.58433	0.51724E-01	0.12437E-03
12	0.74170E-11	0.11148	0.83199	0.56503E-01	0.26336E-04

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

STAGE	WATER
1	0.72117E-08
2	0.50575E-09
3	0.13796E-09
4	0.11800E-09
5	0.11714E-09
6	0.11719E-09
7	0.81217E-11
11	0.12479E-15
12	0.51433E-17

**** MASS-Y-PROFILE ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01

1	0.43038E-01	0.95460	0.14905E-05	0.31091E-07	0.23581E-02
2	0.39881E-02	0.99401	0.78505E-05	0.19710E-06	0.19893E-02
3	0.11437E-02	0.99711	0.32123E-04	0.96870E-06	0.17150E-02
4	0.93001E-03	0.99741	0.12596E-03	0.45847E-05	0.15306E-02
5	0.91415E-03	0.99717	0.48801E-03	0.21494E-04	0.14084E-02
6	0.91352E-03	0.99578	0.18793E-02	0.10020E-03	0.13263E-02
7	0.86185E-04	0.99632	0.23721E-02	0.12923E-03	0.10970E-02
11	0.50199E-08	0.73696	0.23852	0.24167E-01	0.35213E-03
12	0.23533E-09	0.36613	0.58207	0.51680E-01	0.12526E-03

**** MASS-Y-PROFILE ****

STAGE	WATER
1	0.10767E-06
2	0.74110E-08
3	0.20188E-08
4	0.17226E-08
5	0.17066E-08
6	0.17068E-08
7	0.11812E-09
11	0.24423E-14
12	0.12588E-15

****
***** HYDRAULIC PARAMETERS *****
****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE

RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

	TEMPERATURE F	
STAGE	LIQUID FROM	VAPOR TO
1	377.14	386.93
2	386.93	387.65
3	387.65	388.17
4	388.17	388.74
5	388.74	389.56
6	389.56	390.19
7	390.22	391.28
11	437.24	476.10
12	476.10	476.10

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	0.32996E+06	0.33061E+06	5742.2	0.14049E+07	94.059	94.057
2	0.27047E+06	0.33659E+06	4731.8	0.14208E+07	94.124	94.110
3	0.27062E+06	0.33674E+06	4736.1	0.14124E+07	94.128	94.113
4	0.27061E+06	0.33673E+06	4737.2	0.14036E+07	94.134	94.118
5	0.27042E+06	0.33654E+06	4734.3	0.13943E+07	94.158	94.137
6	0.33922E+06	0.33696E+06	5935.8	0.13969E+07	94.258	94.157
7	0.33899E+06	0.33631E+06	5932.2	0.13767E+07	94.292	94.193
11	0.29623E+06	0.29354E+06	4882.3	0.11692E+07	104.20	104.16
12	2684.5	0.0000	43.497	0.0000	108.66	

	DENSITY LB/CUFT		VISCOSITY CP		SURFACE TENSION DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	57.461	0.23532	0.16327	0.11378E-01	21.170
2	57.160	0.23691	0.15058	0.11386E-01	20.653
3	57.140	0.23841	0.14971	0.11393E-01	20.616
4	57.126	0.23991	0.14915	0.11401E-01	20.591
5	57.120	0.24136	0.14880	0.11412E-01	20.573
6	57.147	0.24122	0.14918	0.11419E-01	20.583
7	57.145	0.24429	0.14884	0.11434E-01	20.567

11	60.674	0.25106	0.27505	0.12198E-01	23.003
12	61.716		0.35954		23.062

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.63868E-01	90092.	0.68153E+06
2	-.51742	0.51732E-01	91657.	0.69153E+06
3	-.36844E-01	0.51911E-01	91425.	0.68965E+06
4	-.25443E-01	0.52080E-01	91151.	0.68748E+06
5	-.17966E-01	0.52233E-01	90830.	0.68502E+06
6	-.48237E-01	0.65405E-01	90947.	0.68607E+06
7	-.16217E-01	0.65904E-01	90205.	0.68044E+06
11	1.2932	0.64915E-01	75367.	0.58584E+06
12	0.58492E-01		0.0000	0.0000

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		5
FLOODING CALCULATION METHOD		GLITSCH6
DESIGN PARAMETERS		
PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		2
TRAY SPACING	FT	1.50000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		4
COLUMN DIAMETER	FT	11.6265
DC AREA/COLUMN AREA		0.087500
SIDE DOWNCOMER VELOCITY	FT/SEC	0.14165
FLOW PATH LENGTH	FT	4.22485
SIDE DOWNCOMER WIDTH	FT	1.13135
SIDE WEIR LENGTH	FT	6.89165
CENTER DOWNCOMER WIDTH	FT	0.91409
CENTER WEIR LENGTH	FT	11.5905
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	MISSING
OFF-CENTER LONG WEIR LENGTH	FT	MISSING
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
2	11.626	106.17	42.467	4.6448
3	11.626	106.17	42.467	4.6448
4	11.626	106.17	42.467	4.6448
5	11.626	106.17	42.467	4.6448

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP	DC BACKUP	DC BACKUP/ (TSPC+WHT)
		PSI	FT	
2	0.8039	0.1352	0.7192	0.4426
3	0.8022	0.1347	0.7177	0.4416
4	0.8000	0.1341	0.7157	0.4404

5	0.7974	0.1335	0.7133	0.4389

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.2469	0.6082	0.1774	0.4939
3	0.2469	0.6082	0.1776	0.4929
4	0.2467	0.6082	0.1778	0.4916
5	0.2464	0.6082	0.1781	0.4900

****
*** SECTION 2 ***
****

STARTING STAGE NUMBER		6
ENDING STAGE NUMBER		11
FLOODING CALCULATION METHOD		GLITSCH6

DESIGN PARAMETERS

PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000
MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		2
TRAY SPACING	FT	1.50000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		6
COLUMN DIAMETER	FT	11.7430
DC AREA/COLUMN AREA		0.087500
SIDE DOWNCOMER VELOCITY	FT/SEC	0.17399

FLOW PATH LENGTH	FT	4.26718
SIDE DOWNCOMER WIDTH	FT	1.14269
SIDE WEIR LENGTH	FT	6.96069
CENTER DOWNCOMER WIDTH	FT	0.92324
CENTER WEIR LENGTH	FT	11.7066
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	MISSING
OFF-CENTER LONG WEIR LENGTH	FT	MISSING
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
6	11.743	108.30	43.322	4.7383
7	11.743	108.30	43.322	4.7383
8	11.743	108.30	43.322	4.7383
9	11.743	108.30	43.322	4.7383
10	11.743	108.30	43.322	4.7383
11	11.743	108.30	43.322	4.7383

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
6	0.8000	0.1326	0.7528	0.4633
7	0.7942	0.1312	0.7477	0.4601
8	0.7882	0.1299	0.7413	0.4562
9	0.7691	0.1265	0.7205	0.4434
10	0.7187	0.1183	0.6680	0.4111
11	0.6626	0.1110	0.6156	0.3788

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
6	0.2837	0.6082	0.1795	0.4814
7	0.2829	0.6082	0.1801	0.4776
8	0.2811	0.6082	0.1807	0.4755

```
  9    0.2742      0.6082      0.1825      0.4620
 10    0.2555      0.6082      0.1877      0.4293
 11    0.2356      0.6082      0.1942      0.3933

BLOCK:  T-402    MODEL: RADFRAC
------------------------------
   INLETS    - 26       STAGE  15
   OUTLETS   - 28       STAGE   1
               30       STAGE  20
               29       STAGE  18
  PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN               OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(LBMOL/HR)            695.970          695.970        0.326700E-15
      MASS(LB/HR    )           65462.2          65462.2        0.469109E-11
      ENTHALPY(BTU/HR  )     -0.358074E+08    -0.223126E+08    -0.376872

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



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

  ****    INPUT PARAMETERS    ****

   NUMBER OF STAGES                                        20
   ALGORITHM OPTION                                    STANDARD
   ABSORBER OPTION                                     NO
   INITIALIZATION OPTION                               STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                    NO
   INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
   DESIGN SPECIFICATION METHOD                         NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS              25
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MAXIMUM NO. OF INSIDE LOOP ITERATIONS		10
MAXIMUM NUMBER OF FLASH ITERATIONS		30
FLASH TOLERANCE		0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE		0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST		0.0
MOLAR REFLUX RATIO		20.0000
MOLAR DISTILLATE RATE	LBMOL/HR	23.5000

**** PROFILES ****

P-SPEC	STAGE 1	PRES, PSIA	20.0000

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

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS		
	28	30	29
COMPONENT:			
BENZENE	.99740	.17217E-08	.25953E-02
PHENOL	.28935E-01	.67867E-03	.97039
CATECHOL	.68509E-11	.64746E-01	.93525
BENZO-01	.42883E-12	.11120	.88880
BENZA-01	.18249	.33649E-03	.81717
WATER	.99901	.24880E-09	.98804E-03

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	303.610
BOTTOM STAGE TEMPERATURE	F	395.570
TOP STAGE LIQUID FLOW	LBMOL/HR	687.421
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	0.47000
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	1,500.05

MOLAR REFLUX RATIO		29.2519
MOLAR BOILUP RATIO		3,191.59
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.154942+08
REBOILER DUTY	BTU/HR	0.289890+08

**** MANIPULATED VARIABLES ****

	BOUNDS		CALCULATED
	LOWER	UPPER	VALUE
MOLAR REFLUX RATIO	1.0000	1000.0	29.252

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MASS-FRAC	STREAMS: 29 COMPS: PHENOL		0.99830	0.99830

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

DEW POINT	0.48926E-05	STAGE= 1	
BUBBLE POINT	0.79140E-05	STAGE= 1	
COMPONENT MASS BALANCE	0.22063E-05	STAGE= 15	COMP=BENZENE
ENERGY BALANCE	0.24607E-05	STAGE= 1	

**** PROFILES ****

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

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	ENTHALPY BTU/LBMOL VAPOR	HEAT DUTY BTU/HR
1	303.61	20.000	-43346.	21507.	-.15494+08
2	377.33	22.000	-50434.	-21552.	
14	392.54	23.800	-51027.	-31365.	
15	392.99	23.950	-51007.	-31353.	
16	393.69	24.100	-51004.	-31613.	
17	394.19	24.250	-50989.	-31651.	

18	394.64	24.400	-50976.	-31652.	
19	395.10	24.550	-50968.	-31645.	
20	395.57	24.700	-50991.	-31642.	.28989+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	710.9	0.000				23.5000	
2	758.0	710.9					
14	773.2	796.5					
15	1497.	796.7	695.9700				
16	1498.	824.1					
17	1500.	825.9					
18	1500.	1499.					672.0000
19	1501.	1500.					
20	0.4700	1500.				0.4700	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.6541E+05	0.000				2162.0477	
2	0.7125E+05	0.6541E+05					
14	0.7278E+05	0.7492E+05					
15	0.1409E+06	0.7494E+05	.65462+05				
16	0.1410E+06	0.7757E+05					
17	0.1412E+06	0.7774E+05					
18	0.1412E+06	0.1411E+06					.63256+05
19	0.1412E+06	0.1412E+06					
20	44.24	0.1412E+06				44.2432	

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.13909	0.85138	0.13628E-14	0.19311E-17	0.95256E-02
2	0.14109E-01	0.97697	0.78379E-14	0.13519E-16	0.89219E-02
14	0.43972E-03	0.99769	0.78517E-06	0.14191E-07	0.18683E-02
15	0.44101E-03	0.99780	0.35847E-05	0.78928E-07	0.17565E-02
16	0.77049E-04	0.99827	0.39132E-05	0.84969E-07	0.16513E-02
17	0.12652E-04	0.99849	0.67058E-05	0.14777E-06	0.14915E-02
18	0.12401E-05	0.99872	0.30241E-04	0.79332E-06	0.12495E-02
19	0.12187E-06	0.99881	0.13936E-03	0.44443E-05	0.10474E-02

20	0.12005E-07	0.99845	0.64398E-03	0.25039E-04	0.87820E-03

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

STAGE	WATER
1	0.11140E-05
2	0.82140E-07
14	0.24843E-08
15	0.24901E-08
16	0.31720E-09
17	0.38517E-10
18	0.27339E-11
19	0.19452E-12
20	0.13872E-13

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.74159	0.25454	0.58269E-16	0.65885E-19	0.38616E-02
2	0.13909	0.85138	0.13628E-14	0.19311E-17	0.95256E-02
14	0.45294E-02	0.99324	0.16653E-06	0.24714E-08	0.22293E-02
15	0.45293E-02	0.99338	0.76201E-06	0.13772E-07	0.20942E-02
16	0.79054E-03	0.99724	0.83740E-06	0.14920E-07	0.19730E-02
17	0.12949E-03	0.99809	0.14393E-05	0.26017E-07	0.17816E-02
18	0.12656E-04	0.99849	0.65060E-05	0.13997E-06	0.14917E-02
19	0.12404E-05	0.99872	0.30049E-04	0.78572E-06	0.12496E-02
20	0.12190E-06	0.99881	0.13920E-03	0.44378E-05	0.10475E-02

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

STAGE	WATER
1	0.84076E-05
2	0.11140E-05
14	0.35275E-07
15	0.35270E-07
16	0.44906E-08
17	0.54413E-09
18	0.38529E-10
19	0.27348E-11
20	0.19458E-12

**** K-VALUES ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	5.3319	0.29897	0.42756E-01	0.34117E-01	0.40539
2	9.8583	0.87145	0.17387	0.14285	1.0677

14	10.301	0.99554	0.21210	0.17416	1.1932
15	10.270	0.99557	0.21258	0.17449	1.1922
16	10.260	0.99897	0.21399	0.17559	1.1948
17	10.234	0.99960	0.21464	0.17607	1.1945
18	10.206	0.99977	0.21514	0.17643	1.1938
19	10.178	0.99991	0.21562	0.17679	1.1930
20	10.155	1.0004	0.21616	0.17723	1.1928

**** K-VALUES ****

STAGE	WATER
1	7.5472
2	13.562
14	14.199
15	14.164
16	14.157
17	14.127
18	14.093
19	14.059
20	14.027

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

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.11809	0.87092	0.16311E-14	0.25634E-17	0.10988E-01
2	0.11725E-01	0.97820	0.91820E-14	0.17564E-16	0.10073E-01
14	0.36491E-03	0.99753	0.91850E-06	0.18411E-07	0.21064E-02
15	0.36598E-03	0.99765	0.41935E-05	0.10240E-06	0.19804E-02
16	0.63938E-04	0.99807	0.45775E-05	0.11024E-06	0.18617E-02
17	0.10499E-04	0.99830	0.78443E-05	0.19172E-06	0.16815E-02
18	0.10291E-05	0.99855	0.35376E-04	0.10293E-05	0.14088E-02
19	0.10114E-06	0.99865	0.16302E-03	0.57661E-05	0.11809E-02
20	0.99615E-08	0.99822	0.75328E-03	0.32484E-04	0.99005E-03

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

STAGE	WATER
1	0.21814E-06
2	0.15743E-07
14	0.47547E-09
15	0.47659E-09
16	0.60708E-10
17	0.73717E-11
18	0.52325E-12
19	0.37230E-13

20	0.26548E-14

**** MASS-Y-PROFILE ****

STAGE	BENZENE	PHENOL	CATECHOL	BENZO-01	BENZA-01
1	0.70392	0.29110	0.77966E-16	0.97772E-19	0.49798E-02
2	0.11809	0.87092	0.16311E-14	0.25634E-17	0.10988E-01
14	0.37612E-02	0.99372	0.19494E-06	0.32084E-08	0.25150E-02
15	0.37612E-02	0.99388	0.89201E-06	0.17880E-07	0.23626E-02
16	0.65607E-03	0.99712	0.97964E-06	0.19358E-07	0.22246E-02
17	0.10745E-03	0.99788	0.16836E-05	0.33754E-07	0.20086E-02
18	0.10503E-04	0.99830	0.76105E-05	0.18159E-06	0.16817E-02
19	0.10294E-05	0.99855	0.35151E-04	0.10194E-05	0.14089E-02
20	0.10116E-06	0.99865	0.16284E-03	0.57577E-05	0.11810E-02

**** MASS-Y-PROFILE ****

STAGE	WATER
1	0.18406E-05
2	0.21814E-06
14	0.67557E-08
15	0.67548E-08
16	0.85950E-09
17	0.10414E-09
18	0.73740E-11
19	0.52341E-12
20	0.37241E-13

****
***** HYDRAULIC PARAMETERS *****
****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE

SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

	TEMPERATURE F	
STAGE	LIQUID FROM	VAPOR TO
1	303.61	377.33
2	377.33	386.44
14	392.54	392.99
15	392.99	393.69
16	393.69	394.19
17	394.19	394.64
18	394.64	395.10
19	395.10	395.57
20	395.57	395.57

	MASS FLOW LB/HR		VOLUME FLOW CUFT/HR		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	65406.	65406.	1125.0	0.28114E+06	92.002	92.002
2	71245.	73407.	1243.9	0.31000E+06	93.994	93.935
14	72782.	74944.	1278.1	0.29394E+06	94.128	94.066
15	0.14087E+06	77569.	2474.4	0.30234E+06	94.127	94.124
16	0.14104E+06	77743.	2478.4	0.30124E+06	94.132	94.132
17	0.14116E+06	77856.	2481.1	0.29994E+06	94.131	94.131
18	0.14120E+06	0.14116E+06	2482.6	0.54069E+06	94.129	94.129
19	0.14124E+06	0.14120E+06	2484.0	0.53776E+06	94.128	94.128
20	44.243	0.0000	0.77826	0.0000	94.135	

	DENSITY LB/CUFT		VISCOSITY CP		SURFACE TENSION DYNE/CM
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	58.138	0.23265	0.29575	0.11317E-01	23.269
2	57.276	0.23680	0.16324	0.11373E-01	20.520
14	56.946	0.25497	0.14383	0.11463E-01	20.341

15	56.930	0.25656	0.14329	0.11470E-01	20.316
16	56.909	0.25808	0.14247	0.11477E-01	20.280
17	56.892	0.25957	0.14188	0.11484E-01	20.253
18	56.876	0.26107	0.14134	0.11490E-01	20.228
19	56.861	0.26256	0.14082	0.11497E-01	20.204
20	56.849		0.14038		20.182

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR CUFT/HR	REDUCED F-FACTOR (LB-CUFT)**.5/HR
1		0.63259E-01	17820.	0.13560E+06
2	-2.7484	0.62405E-01	19974.	0.15085E+06
14	0.12604	0.64982E-01	19712.	0.14842E+06
15	-.41302	0.12191	20343.	0.15314E+06
16	-.36557E-01	0.12217	20332.	0.15303E+06
17	-.26791E-01	0.12247	20306.	0.15281E+06
18	-.24862E-01	0.67772E-01	36716.	0.27627E+06
19	-.23991E-01	0.67974E-01	36627.	0.27555E+06
20	-.21908E-01		0.0000	0.0000

****
***** TRAY SIZING CALCULATIONS *****
****

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		14
FLOODING CALCULATION METHOD		GLITSCH6
DESIGN PARAMETERS		
PEAK CAPACITY FACTOR		1.00000
SYSTEM FOAMING FACTOR		1.00000
FLOODING FACTOR		0.80000
MINIMUM COLUMN DIAMETER	FT	1.00000

MINIMUM DC AREA/COLUMN AREA		0.100000
HOLE AREA/ACTIVE AREA		0.100000

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		2
TRAY SPACING	FT	1.50000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		14
COLUMN DIAMETER	FT	5.31004
DC AREA/COLUMN AREA		0.087500
SIDE DOWNCOMER VELOCITY	FT/SEC	0.18322
FLOW PATH LENGTH	FT	1.92957
SIDE DOWNCOMER WIDTH	FT	0.51671
SIDE WEIR LENGTH	FT	3.14755
CENTER DOWNCOMER WIDTH	FT	0.41748
CENTER WEIR LENGTH	FT	5.29361
OFF-CENTER DOWNCOMER WIDTH	FT	0.0
OFF-CENTER SHORT WEIR LENGTH	FT	MISSING
OFF-CENTER LONG WEIR LENGTH	FT	MISSING
TRAY CENTER TO OCDC CENTER	FT	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
2	5.3100	22.146	8.8582	0.96887
3	5.3100	22.146	8.8582	0.96887
4	5.3100	22.146	8.8582	0.96887
5	5.3100	22.146	8.8582	0.96887
6	5.3100	22.146	8.8582	0.96887
7	5.3100	22.146	8.8582	0.96887
8	5.3100	22.146	8.8582	0.96887
9	5.3100	22.146	8.8582	0.96887
10	5.3100	22.146	8.8582	0.96887
11	5.3100	22.146	8.8582	0.96887

12	5.3100	22.146	8.8582	0.96887
13	5.3100	22.146	8.8582	0.96887
14	5.3100	22.146	8.8582	0.96887

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
2	0.8086	0.1395	0.6735	0.4145
3	0.8203	0.1421	0.6859	0.4221
4	0.8195	0.1418	0.6851	0.4216
5	0.8174	0.1412	0.6830	0.4203
6	0.8154	0.1406	0.6809	0.4190
7	0.8133	0.1400	0.6789	0.4178
8	0.8113	0.1395	0.6769	0.4165
9	0.8094	0.1389	0.6749	0.4153
10	0.8074	0.1384	0.6730	0.4141
11	0.8055	0.1378	0.6711	0.4130
12	0.8037	0.1374	0.6696	0.4120
13	0.8018	0.1369	0.6678	0.4109
14	0.8000	0.1364	0.6661	0.4099

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.1744	0.6082	0.1743	0.5175
3	0.1773	0.6082	0.1735	0.5279
4	0.1775	0.6082	0.1735	0.5277
5	0.1774	0.6082	0.1737	0.5265
6	0.1774	0.6082	0.1739	0.5253
7	0.1773	0.6082	0.1741	0.5241
8	0.1772	0.6082	0.1743	0.5229
9	0.1772	0.6082	0.1745	0.5217
10	0.1771	0.6082	0.1746	0.5206
11	0.1771	0.6082	0.1748	0.5195
12	0.1770	0.6082	0.1750	0.5152
13	0.1770	0.6082	0.1752	0.5141
14	0.1769	0.6082	0.1754	0.5121

```
********************
*** SECTION   2 ***
********************

STARTING STAGE NUMBER                                    15
ENDING STAGE NUMBER                                      19
FLOODING CALCULATION METHOD                          GLITSCH6

DESIGN PARAMETERS
-----------------
PEAK CAPACITY FACTOR                                 1.00000
SYSTEM FOAMING FACTOR                                1.00000
FLOODING FACTOR                                      0.80000
MINIMUM COLUMN DIAMETER          FT                  1.00000
MINIMUM DC AREA/COLUMN AREA                          0.100000
HOLE AREA/ACTIVE AREA                                0.100000

TRAY SPECIFICATIONS
-------------------
TRAY TYPE                                            SIEVE
NUMBER OF PASSES                                         2
TRAY SPACING                     FT                  1.50000


        ***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER                              19
COLUMN DIAMETER                  FT                  7.31726
DC AREA/COLUMN AREA                                  0.087500
SIDE DOWNCOMER VELOCITY          FT/SEC              0.18752
FLOW PATH LENGTH                 FT                  2.65896
SIDE DOWNCOMER WIDTH             FT                  0.71203
SIDE WEIR LENGTH                 FT                  4.33734
CENTER DOWNCOMER WIDTH           FT                  0.57529
CENTER WEIR LENGTH               FT                  7.29461
OFF-CENTER DOWNCOMER WIDTH       FT                  0.0
OFF-CENTER SHORT WEIR LENGTH     FT                  MISSING
OFF-CENTER LONG WEIR LENGTH      FT                  MISSING
TRAY CENTER TO OCDC CENTER       FT                  0.0
```

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	FT	SQFT	SQFT	SQFT
15	7.3173	42.052	16.821	1.8398
16	7.3173	42.052	16.821	1.8398
17	7.3173	42.052	16.821	1.8398
18	7.3173	42.052	16.821	1.8398
19	7.3173	42.052	16.821	1.8398

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP PSI	DC BACKUP FT	DC BACKUP/ (TSPC+WHT)
15	0.4687	0.7572E-01	0.4981	0.3065
16	0.4686	0.7570E-01	0.4983	0.3067
17	0.4682	0.7564E-01	0.4984	0.3067
18	0.8018	0.1351	0.6945	0.4274
19	0.8000	0.1347	0.6929	0.4264

STAGE	HEIGHT OVER WEIR FT	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
15	0.1728	0.6082	0.2524	0.2784
16	0.1730	0.6082	0.2525	0.2784
17	0.1730	0.6082	0.2528	0.2782
18	0.2207	0.6082	0.1768	0.5032
19	0.2206	0.6082	0.1769	0.5021

Appendix 5.4: Stream Results

1 10 11 12 13

STREAM ID	1	10	11	12	13
FROM :	----	DUMMY	DUMMY	C-301	P-301
TO :	C-E101-3	C-301	P-301	E-301	E-303
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	LIQUID	MIXED	LIQUID
COMPONENTS: LBMOL/HR					
BENZENE	0.0	1785.0076	3287.0474	1785.0076	3287.0474
PHENOL	0.0	92.8972	608.5062	92.8972	608.5062
CATECHOL	0.0	1.3350	18.9532	1.3350	18.9532
BENZO-01	0.0	5.1005-02	1.1911	5.1005-02	1.1911
BENZA-01	0.0	0.1465	1.0957	0.1465	1.0957
WATER	0.0	8.7700	8.0781	8.7700	8.0781
OXYGEN	410.0000	33.5190	3.2265	33.5190	3.2265
NITROGEN	1551.1330	1459.2269	93.1409	1459.2269	93.1409
COMPONENTS: LB/HR					
BENZENE	0.0	1.3943+05	2.5676+05	1.3943+05	2.5676+05
PHENOL	0.0	8742.8368	5.7268+04	8742.8368	5.7268+04
CATECHOL	0.0	146.9987	2086.9867	146.9987	2086.9867
BENZO-01	0.0	6.2290	145.4650	6.2290	145.4650
BENZA-01	0.0	15.5452	116.2773	15.5452	116.2773
WATER	0.0	157.9947	145.5297	157.9947	145.5297
OXYGEN	1.3120+04	1072.5669	103.2448	1072.5669	103.2448
NITROGEN	4.3453+04	4.0878+04	2609.2010	4.0878+04	2609.2010
COMPONENTS: STD CUFT/HR					
BENZENE	0.0	2530.7477	4660.3094	2530.7477	4660.3094
PHENOL	0.0	133.5053	874.5026	133.5053	874.5026
CATECHOL	0.0	1.9086	27.0966	1.9086	27.0966
BENZO-01	0.0	8.4156-02	1.9653	8.4156-02	1.9653
BENZA-01	0.0	0.2391	1.7883	0.2391	1.7883
WATER	0.0	2.5357	2.3357	2.5357	2.3357
OXYGEN	351.7446	28.7564	2.7681	28.7564	2.7681
NITROGEN	1330.7382	1251.8907	79.9069	1251.8907	79.9069
TOTAL CUFT/HR	1682.4828	3949.6676	5650.6727	3949.6676	5650.6727
TOTAL FLOW:					
LBMOL/HR	1961.1330	3380.9532	4021.2392	3380.9532	4021.2392
LB/HR	5.6572+04	1.9045+05	3.1924+05	1.9045+05	3.1924+05
CUFT/HR	7.8084+05	4.7368+04	7892.3092	1.5263+05	7838.2381

STATE VARIABLES:					
TEMP F	86.0000	441.4811	441.4811	327.4897	436.9785
PRES PSIA	14.7000	590.3676	590.3676	169.7359	169.7359
VFRAC	1.0000	1.0000	0.0	0.9662	0.0
LFRAC	0.0	0.0	1.0000	3.3783-02	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	59.3305	2.3049+04	2.0954+04	2.0855+04	2.0862+04
BTU/LB	2.0568	409.1697	263.9442	370.2126	262.7896
BTU/HR	1.1636+05	7.7928+07	8.4261+07	7.0508+07	8.3893+07
ENTROPY:					
BTU/LBMOL-R	1.1283	-18.3342	-41.4002	-18.7511	-41.3365
BTU/LB-R	3.9113-02	-0.3255	-0.5215	-0.3329	-0.5207
DENSITY:					
LBMOL/CUFT	2.5116-03	7.1377-02	0.5095	2.2151-02	0.5130
LB/CUFT	7.2450-02	4.0207	40.4493	1.2478	40.7283
AVG MW	28.8467	56.3313	79.3880	56.3313	79.3880

14 15 16 17 18

STREAM ID	14	15	16	17	18
FROM :	E-301	E-303	E-302	E-304	T-301
TO :	E-302	E-304	T-301	T-301	----
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	MIXED	MIXED	VAPOR
COMPONENTS: LBMOL/HR					
BENZENE	1785.0076	3287.0474	1785.0076	3287.0474	41.3940
PHENOL	92.8972	608.5062	92.8972	608.5062	9.7492-02
CATECHOL	1.3350	18.9532	1.3350	18.9532	1.7549-04
BENZO-01	5.1005-02	1.1911	5.1005-02	1.1911	4.3726-06
BENZA-01	0.1465	1.0957	0.1465	1.0957	2.3790-04
WATER	8.7700	8.0781	8.7700	8.0781	0.4422
OXYGEN	33.5190	3.2265	33.5190	3.2265	34.6361
NITROGEN	1459.2269	93.1409	1459.2269	93.1409	1522.7118
COMPONENTS: LB/HR					
BENZENE	1.3943+05	2.5676+05	1.3943+05	2.5676+05	3233.4373
PHENOL	8742.8368	5.7268+04	8742.8368	5.7268+04	9.1753
CATECHOL	146.9987	2086.9867	146.9987	2086.9867	1.9324-02
BENZO-01	6.2290	145.4650	6.2290	145.4650	5.3399-04
BENZA-01	15.5452	116.2773	15.5452	116.2773	2.5247-02

WATER	157.9947	145.5297	157.9947	145.5297	7.9668
OXYGEN	1072.5669	103.2448	1072.5669	103.2448	1108.3138
NITROGEN	4.0878+04	2609.2010	4.0878+04	2609.2010	4.2656+04
COMPONENTS: STD CUFT/HR					
BENZENE	2530.7477	4660.3094	2530.7477	4660.3094	58.6876
PHENOL	133.5053	874.5026	133.5053	874.5026	0.1401
CATECHOL	1.9086	27.0966	1.9086	27.0966	2.5089-04
BENZO-01	8.4156-02	1.9653	8.4156-02	1.9653	7.2144-06
BENZA-01	0.2391	1.7883	0.2391	1.7883	3.8830-04
WATER	2.5357	2.3357	2.5357	2.3357	0.1279
OXYGEN	28.7564	2.7681	28.7564	2.7681	29.7148
NITROGEN	1251.8907	79.9069	1251.8907	79.9069	1306.3552
TOTAL CUFT/HR	3949.6676	5650.6727	3949.6676	5650.6727	1395.0262
TOTAL FLOW:					
LBMOL/HR	3380.9532	4021.2392	3380.9532	4021.2392	1599.2820
LB/HR	1.9045+05	3.1924+05	1.9045+05	3.1924+05	4.7015+04
CUFT/HR	1.1896+05	1.2243+04	6.0759+04	8668.4222	6.0919+04
STATE VARIABLES:					
TEMP F	285.0000	285.0000	110.0000	110.0000	110.1187
PRES PSIA	164.7359	164.7359	159.7359	159.7359	159.7359
VFRAC	0.7484	3.0987-02	0.4510	1.9248-02	1.0000
LFRAC	0.2516	0.9690	0.5490	0.9808	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	1.7417+04	1.4166+04	1.0074+04	7940.5322	1093.8012
BTU/LB	309.1973	178.4419	178.8370	100.0218	37.2069
BTU/HR	5.8888+07	5.6965+07	3.4060+07	3.1931+07	1.7493+06
ENTROPY:					
BTU/LBMOL-R	-23.1945	-49.4375	-34.0915	-58.9032	-4.8828
BTU/LB-R	-0.4118	-0.6227	-0.6052	-0.7420	-0.1661
DENSITY:					
LBMOL/CUFT	2.8422-02	0.3285	5.5645-02	0.4639	2.6253-02
LB/CUFT	1.6010	26.0753	3.1346	36.8277	0.7718
AVG MW	56.3313	79.3880	56.3313	79.3880	29.3978

19 2 20 21 22

STREAM ID	19	2	20	21	22
FROM :	T-301	C-E101-3	T-302	T-302	P-102
TO :	T-302	DUMMIX	----	P-102	MIX

CONV. MAX. REL. ERR:	0.0	0.0	0.0	9.6468-05	0.0
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
BENZENE	5030.6610	0.0	70.3880	4956.6335	4956.6335
PHENOL	701.3059	0.0	6.0247-06	1.0632-02	1.0632-02
CATECHOL	20.2880	0.0	1.5873-12	2.3181-08	2.3181-08
BENZO-01	1.2421	0.0	3.6409-16	1.4134-11	1.4134-11
BENZA-01	1.2419	0.0	1.1824-08	1.9761-05	1.9761-05
WATER	16.4059	0.0	0.7997	15.6047	15.6047
OXYGEN	2.1094	410.0000	1.8950	0.2144	0.2144
NITROGEN	29.6561	1551.1330	28.4213	1.2348	1.2348
COMPONENTS: LB/HR					
BENZENE	3.9296+05	0.0	5498.2647	3.8718+05	3.8718+05
PHENOL	6.6002+04	0.0	5.6700-04	1.0006	1.0006
CATECHOL	2233.9661	0.0	1.7478-10	2.5526-06	2.5526-06
BENZO-01	151.6934	0.0	4.4464-14	1.7261-09	1.7261-09
BENZA-01	131.7973	0.0	1.2548-06	2.0971-03	2.0971-03
WATER	295.5576	0.0	14.4074	281.1226	281.1226
OXYGEN	67.4979	1.3120+04	60.6387	6.8593	6.8593
NITROGEN	830.7698	4.3453+04	796.1795	34.5919	34.5919
COMPONENTS: STD CUFT/HR					
BENZENE	7132.3694	0.0	99.7947	7027.4148	7027.4148
PHENOL	1007.8678	0.0	8.6583-06	1.5279-02	1.5279-02
CATECHOL	29.0049	0.0	2.2693-12	3.3141-08	3.3141-08
BENZO-01	2.0494	0.0	6.0073-16	2.3320-11	2.3320-11
BENZA-01	2.0270	0.0	1.9299-08	3.2254-05	3.2254-05
WATER	4.7435	0.0	0.2312	4.5118	4.5118
OXYGEN	1.8097	351.7446	1.6258	0.1839	0.1839
NITROGEN	25.4423	1330.7382	24.3830	1.0594	1.0594
TOTAL CUFT/HR	8205.3141	1682.4828	126.0347	7033.1852	7033.1852
TOTAL FLOW:					
LBMOL/HR	5802.9104	1961.1330	101.5041	4973.6981	4973.6981
LB/HR	4.6268+05	5.6572+04	6369.4909	3.8750+05	3.8750+05
CUFT/HR	8422.6335	3.0162+04	3.3696+04	7596.8831	7620.9236
STATE VARIABLES:					
TEMP F	110.1187	384.0399	172.4085	172.4085	176.6281
PRES PSIA	159.7359	594.8469	20.0000	20.0000	652.8620
VFRAC	0.0	1.0000	1.0000	0.0	0.0
LFRAC	1.0000	0.0	0.0	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0

ENTHALPY:					
BTU/LBMOL	1.1071+04	2115.9554	2.5454+04	2.4032+04	2.4266+04
BTU/LB	138.8478	73.3518	405.6273	308.4602	311.4557
BTU/HR	6.4242+07	4.1497+06	2.5836+06	1.1953+08	1.2069+08
ENTROPY:					
BTU/LBMOL-R	-59.3115	-3.2234	-22.4869	-54.4916	-54.3948
BTU/LB-R	-0.7439	-0.1117	-0.3584	-0.6994	-0.6982
DENSITY:					
LBMOL/CUFT	0.6890	6.5019-02	3.0123-03	0.6547	0.6526
LB/CUFT	54.9325	1.8756	0.1890	51.0083	50.8474
AVG MW	79.7318	28.8467	62.7511	77.9107	77.9107

23 24 25 26 27

STREAM ID	23	24	25	26	27
FROM :	T-302	T-401	T-401	P-403	T-401
TO :	T-401	----	P-403	T-402	PRODMIX
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
BENZENE	3.6385	0.3614	3.2771	3.2771	2.5489-10
PHENOL	701.2953	6.6540	691.4614	691.4614	3.1798
CATECHOL	20.2880	8.8797-06	4.6747-03	4.6747-03	20.2834
BENZO-01	1.2421	1.6701-07	1.0583-04	1.0583-04	1.2420
BENZA-01	1.2419	1.4577-02	1.2267	1.2267	6.6620-04
WATER	3.0126-05	3.9205-06	2.6205-05	2.6205-05	7.6640-16
OXYGEN	6.9096-21	0.0	0.0	0.0	0.0
NITROGEN	1.5940-22	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
BENZENE	284.2188	28.2335	255.9853	255.9853	1.9911-08
PHENOL	6.6001+04	626.2252	6.5076+04	6.5076+04	299.2640
CATECHOL	2233.9661	9.7776-04	0.5147	0.5147	2233.4504
BENZO-01	151.6934	2.0396-05	1.2924-02	1.2924-02	151.6804
BENZA-01	131.7952	1.5470	130.1776	130.1776	7.0699-02
WATER	5.4272-04	7.0629-05	4.7210-04	4.7210-04	1.3807-14
OXYGEN	2.2110-19	0.0	0.0	0.0	0.0
NITROGEN	4.4654-21	0.0	0.0	0.0	0.0
COMPONENTS: STD CUFT/HR					
BENZENE	5.1586	0.5124	4.6462	4.6462	3.6138-10
PHENOL	1007.8525	9.5626	993.7200	993.7200	4.5698

CATECHOL	29.0049	1.2695-05	6.6832-03	6.6832-03	28.9982
BENZO-01	2.0494	2.7555-07	1.7461-04	1.7461-04	2.0493
BENZA-01	2.0270	2.3792-02	2.0021	2.0021	1.0874-03
WATER	8.7104-06	1.1336-06	7.5768-06	7.5768-06	2.2159-16
OXYGEN	5.9278-21	0.0	0.0	0.0	0.0
NITROGEN	1.3675-22	0.0	0.0	0.0	0.0
TOTAL CUFT/HR	1046.0925	10.0989	1000.3752	1000.3752	35.6184
TOTAL FLOW:					
LBMOL/HR	727.7059	7.0300	695.9700	695.9700	24.7059
LB/HR	6.8803+04	656.0068	6.5462+04	6.5462+04	2684.4655
CUFT/HR	1201.4259	3063.2011	1139.2401	1139.2979	43.4970
STATE VARIABLES:					
TEMP F	389.7980	377.1415	377.1415	377.2195	476.1046
PRES PSIA	23.4000	20.0000	20.0000	30.0000	23.5000
VFRAC	0.0	1.0000	0.0	0.0	0.0
LFRAC	1.0000	0.0	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-5.3204+04	-2.8365+04	-5.1455+04	-5.1450+04	-1.1780+05
BTU/LB	-562.7231	-303.9735	-547.0486	-546.9930	-1084.1383
BTU/HR	-3.8717+07	-1.9941+05	-3.5811+07	-3.5807+07	-2.9103+06
ENTROPY:					
BTU/LBMOL-R	-60.9374	-37.2247	-61.3953	-61.3923	-71.5214
BTU/LB-R	-0.6445	-0.3989	-0.6527	-0.6527	-0.6582
DENSITY:					
LBMOL/CUFT	0.6057	2.2950-03	0.6109	0.6109	0.5680
LB/CUFT	57.2675	0.2142	57.4613	57.4584	61.7161
AVG MW	94.5474	93.3153	94.0590	94.0590	108.6569

28 29 3 30 31

STREAM ID	28	29	3	30	31
FROM :	T-402	T-402	----	T-402	PRODMIX
TO :	PRODMIX	E-501	P-101	PRODMIX	E-503
SUBSTREAM: MIXED					
PHASE:	LIQUID	VAPOR	LIQUID	LIQUID	MIXED
COMPONENTS: LBMOL/HR					
BENZENE	3.2686	8.5050-03	840.0000	5.6422-09	3.2686
PHENOL	20.0075	670.9846	0.0	0.4693	23.6566
CATECHOL	3.2026-14	4.3720-03	0.0	3.0267-04	20.2837

BENZO-01	4.5381-17	9.4058-05	0.0	1.1768-05	1.2420
BENZA-01	0.2239	1.0024	0.0	4.1275-04	0.2249
WATER	2.6179-05	2.5892-08	0.0	6.5199-15	2.6179-05
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
BENZENE	255.3210	0.6644	6.5615+04	4.4073-07	255.3210
PHENOL	1882.9703	6.3148+04	0.0	44.1647	2226.3990
CATECHOL	3.5265-12	0.4814	0.0	3.3328-02	2233.4837
BENZO-01	5.5421-15	1.1487-02	0.0	1.4372-03	151.6819
BENZA-01	23.7560	106.3778	0.0	4.3803-02	23.8705
WATER	4.7163-04	4.6645-07	0.0	1.1746-13	4.7163-04
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
COMPONENTS: STD CUFT/HR					
BENZENE	4.6341	1.2058-02	1190.9350	7.9993-09	4.6341
PHENOL	28.7534	964.2922	0.0	0.6744	33.9977
CATECHOL	4.5786-14	6.2505-03	0.0	4.3271-04	28.9986
BENZO-01	7.4876-17	1.5519-04	0.0	1.9417-05	2.0493
BENZA-01	0.3654	1.6361	0.0	6.7369-04	0.3671
WATER	7.5693-06	7.4862-09	0.0	1.8851-15	7.5693-06
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
TOTAL CUFT/HR	33.7529	965.9468	1190.9350	0.6755	70.0469
TOTAL FLOW:					
LBMOL/HR	23.5000	672.0000	840.0000	0.4700	48.6759
LB/HR	2162.0477	6.3256+04	6.5615+04	44.2433	4890.7565
CUFT/HR	37.1883	2.4369+05	1212.1972	0.7783	1877.5220
STATE VARIABLES:					
TEMP F	303.6098	394.6436	86.0000	395.5700	374.4438
PRES PSIA	20.0000	24.4000	14.7000	24.7000	20.0000
VFRAC	0.0	1.0000	0.0	0.0	8.4965-02
LFRAC	1.0000	0.0	1.0000	1.0000	0.9150
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-4.3346+04	-3.1652+04	2.1816+04	-5.0991+04	-8.1209+04
BTU/LB	-471.1437	-336.2528	279.2805	-541.6824	-808.2457
BTU/HR	-1.0186+06	-2.1270+07	1.8325+07	-2.3966+04	-3.9529+06
ENTROPY:					
BTU/LBMOL-R	-62.5358	-37.8774	-59.1454	-60.4451	-65.8772
BTU/LB-R	-0.6797	-0.4024	-0.7572	-0.6421	-0.6557
DENSITY:					

LBMOL/CUFT	0.6319	2.7576-03	0.6930	0.6039	2.5926-02
LB/CUFT	58.1379	0.2596	54.1294	56.8493	2.6049
AVG MW	92.0020	94.1309	78.1136	94.1346	100.4760

32 33 34 35 4

STREAM ID	32	33	34	35	4
FROM :	E-501	E-503	E-502	E-504	P-101
TO :	E-502	E-504	----	----	MIX
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
BENZENE	8.5050-03	3.2686	8.5050-03	3.2686	840.0000
PHENOL	670.9846	23.6566	670.9846	23.6566	0.0
CATECHOL	4.3720-03	20.2837	4.3720-03	20.2837	0.0
BENZO-01	9.4058-05	1.2420	9.4058-05	1.2420	0.0
BENZA-01	1.0024	0.2249	1.0024	0.2249	0.0
WATER	2.5892-08	2.6179-05	2.5892-08	2.6179-05	0.0
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
COMPONENTS: LB/HR					
BENZENE	0.6644	255.3210	0.6644	255.3210	6.5615+04
PHENOL	6.3148+04	2226.3990	6.3148+04	2226.3990	0.0
CATECHOL	0.4814	2233.4837	0.4814	2233.4837	0.0
BENZO-01	1.1487-02	151.6819	1.1487-02	151.6819	0.0
BENZA-01	106.3778	23.8705	106.3778	23.8705	0.0
WATER	4.6645-07	4.7163-04	4.6645-07	4.7163-04	0.0
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
COMPONENTS: STD CUFT/HR					
BENZENE	1.2058-02	4.6341	1.2058-02	4.6341	1190.9350
PHENOL	964.2922	33.9977	964.2922	33.9977	0.0
CATECHOL	6.2505-03	28.9986	6.2505-03	28.9986	0.0
BENZO-01	1.5519-04	2.0493	1.5519-04	2.0493	0.0
BENZA-01	1.6361	0.3671	1.6361	0.3671	0.0
WATER	7.4862-09	7.5693-06	7.4862-09	7.5693-06	0.0
OXYGEN	0.0	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0	0.0
TOTAL CUFT/HR	965.9468	70.0469	965.9468	70.0469	1190.9350
TOTAL FLOW:					

LBMOL/HR	672.0000	48.6759	672.0000	48.6759	840.0000
LB/HR	6.3256+04	4890.7565	6.3256+04	4890.7565	6.5615+04
CUFT/HR	1040.1083	76.7364	953.7617	70.8786	1216.9620
STATE VARIABLES:					
TEMP F	285.0000	285.0000	113.0000	113.0000	92.0649
PRES PSIA	19.4000	15.0000	14.4000	10.0000	652.8620
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-5.6364+04	-8.7194+04	-6.3854+04	-9.5260+04	2.2106+04
BTU/LB	-598.7848	-867.8096	-678.3588	-948.0831	282.9973
BTU/HR	-3.7877+07	-4.2442+06	-4.2910+07	-4.6368+06	1.8569+07
ENTROPY:					
BTU/LBMOL-R	-67.2391	-73.4009	-78.6352	-85.6742	-58.9168
BTU/LB-R	-0.7143	-0.7305	-0.8354	-0.8527	-0.7542
DENSITY:					
LBMOL/CUFT	0.6461	0.6343	0.7046	0.6868	0.6902
LB/CUFT	60.8167	63.7345	66.3226	69.0019	53.9174
AVG MW	94.1309	100.4760	94.1309	100.4760	78.1136

5 6 7 8 9

STREAM ID	5	6	7	8	9
FROM :	MIX	E-201	E-202	DUMMIX	R-201-4
TO :	E-201	E-202	DUMMIX	R-201-4	E-201
CONV. MAX. REL. ERR:	0.0	0.0	0.0	0.0	-8.0278-05
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR
COMPONENTS: LBMOL/HR					
BENZENE	5796.6335	5796.6335	5796.6335	5796.6335	5072.0550
PHENOL	1.0632-02	1.0632-02	1.0632-02	1.0632-02	701.4034
CATECHOL	2.3181-08	2.3181-08	2.3181-08	2.3181-08	20.2882
BENZO-01	1.4134-11	1.4134-11	1.4134-11	1.4134-11	1.2421
BENZA-01	1.9761-05	1.9761-05	1.9761-05	1.9761-05	1.2422
WATER	15.6047	15.6047	15.6047	15.6047	16.8482
OXYGEN	0.2144	0.2144	0.2144	410.2144	36.7455
NITROGEN	1.2348	1.2348	1.2348	1552.3678	1552.3678
COMPONENTS: LB/HR					

BENZENE	4.5280+05	4.5280+05	4.5280+05	4.5280+05	3.9620+05
PHENOL	1.0006	1.0006	1.0006	1.0006	6.6011+04
CATECHOL	2.5526-06	2.5526-06	2.5526-06	2.5526-06	2233.9854
BENZO-01	1.7261-09	1.7261-09	1.7261-09	1.7261-09	151.6939
BENZA-01	2.0971-03	2.0971-03	2.0971-03	2.0971-03	131.8226
WATER	281.1226	281.1226	281.1226	281.1226	303.5244
OXYGEN	6.8593	6.8593	6.8593	1.3126+04	1175.8117
NITROGEN	34.5919	34.5919	34.5919	4.3487+04	4.3487+04
COMPONENTS: STD CUFT/HR					
BENZENE	8218.3498	8218.3498	8218.3498	8218.3498	7191.0570
PHENOL	1.5279-02	1.5279-02	1.5279-02	1.5279-02	1008.0079
CATECHOL	3.3141-08	3.3141-08	3.3141-08	3.3141-08	29.0051
BENZO-01	2.3320-11	2.3320-11	2.3320-11	2.3320-11	2.0494
BENZA-01	3.2254-05	3.2254-05	3.2254-05	3.2254-05	2.0274
WATER	4.5118	4.5118	4.5118	4.5118	4.8714
OXYGEN	0.1839	0.1839	0.1839	351.9285	31.5245
NITROGEN	1.0594	1.0594	1.0594	1331.7976	1331.7976
TOTAL CUFT/HR	8224.1202	8224.1202	8224.1202	9906.6030	9600.3403
TOTAL FLOW:					
LBMOL/HR	5813.6981	5813.6981	5813.6981	7774.8311	7402.1924
LB/HR	4.5312+05	4.5312+05	4.5312+05	5.0969+05	5.0969+05
CUFT/HR	8835.3159	1.4402+04	8.5231+04	1.3889+05	1.2783+05
STATE VARIABLES:					
TEMP F	165.0295	515.4044	698.0000	665.0639	662.0000
PRES PSIA	652.8620	651.1299	646.1299	594.8469	594.8469
VFRAC	0.0	0.0	1.0000	1.0000	1.0000
LFRAC	1.0000	1.0000	0.0	0.0	0.0
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	2.3954+04	3.9151+04	5.2491+04	3.9784+04	3.3847+04
BTU/LB	307.3347	502.3168	673.4755	606.8660	491.5503
BTU/HR	1.3926+08	2.2761+08	3.0517+08	3.0931+08	2.5054+08
ENTROPY:					
BTU/LBMOL-R	-55.0104	-36.1508	-23.2933	-17.0382	-18.7359
BTU/LB-R	-0.7058	-0.4638	-0.2989	-0.2599	-0.2721
DENSITY:					
LBMOL/CUFT	0.6580	0.4037	6.8211-02	5.5978-02	5.7906-02
LB/CUFT	51.2851	31.4618	5.3164	3.6697	3.9872
AVG MW	77.9400	77.9400	77.9400	65.5566	68.8569

DUM

STREAM ID		DUM
FROM :		E-201
TO :		DUMMY
SUBSTREAM: MIXED		
PHASE:		MIXED
COMPONENTS: LBMOL/HR		
BENZENE		5072.0550
PHENOL		701.4034
CATECHOL		20.2882
BENZO-01		1.2421
BENZA-01		1.2422
WATER		16.8482
OXYGEN		36.7455
NITROGEN		1552.3678
COMPONENTS: LB/HR		
BENZENE		3.9620+05
PHENOL		6.6011+04
CATECHOL		2233.9854
BENZO-01		151.6939
BENZA-01		131.8226
WATER		303.5244
OXYGEN		1175.8117
NITROGEN		4.3487+04
COMPONENTS: STD CUFT/HR		
BENZENE		7191.0570
PHENOL		1008.0079
CATECHOL		29.0051
BENZO-01		2.0494
BENZA-01		2.0274
WATER		4.8714
OXYGEN		31.5245
NITROGEN		1331.7976
TOTAL CUFT/HR		9600.3403
TOTAL FLOW:		
LBMOL/HR		7402.1924
LB/HR		5.0969+05
CUFT/HR		5.5260+04
STATE VARIABLES:		
TEMP	F	441.4811
PRES	PSIA	590.3676

VFRAC	0.4567
LFRAC	0.5433
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	2.1911+04
BTU/LB	318.2098
BTU/HR	1.6219+08
ENTROPY:	
BTU/LBMOL-R	-30.8648
BTU/LB-R	-0.4482
DENSITY:	
LBMOL/CUFT	0.1340
LB/CUFT	9.2235
AVG MW	68.8569