Title
Production of 80,000 Mt/year of 99.9 weight% Cumene

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Production of 80,000 Mt/year of 99.9 weight% Cumene

By

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A capstone project submitted for Graduation with University Honors

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University Honors
University of California, Riverside

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Letter of Transmittal

Date: June 4, 2021

To: Professor Sadeddin Kherfan
Bourns College of Engineering
University of California, Riverside

From: Jose Garcia-Torres, Team Leader
Jose Benitez Ponce
Selena Crawford
Giovanna Panelli
Joshua Tai
Jacob Hatt

The group is writing to you with the project report, "Production of 80,000 Mt/year of 99.9 weight% Cumene," enclosed. The purpose of writing this letter is to inform you of the completion of the design, simulation, and optimization of a cumene production process for the assigned CHE 175 Senior Design Project. This project began on January 5, 2021 when the problem statement was assigned and is now completed as of June 4, 2021. The objective of this assignment requested that we choose one of several possible methods to produce cumene, compare and analyze this method versus alternatives, and then create an optimized process. This is a revised edition of the winter report that was previously submitted. In this full report, analysis of profitability and optimization criteria are included. Updates to the Environmental, Health, and Safety section were also made. For perspective, a comparison of the manufacturing costs, amount of materials consumed, and waste produced by the optimized and alternative processes are discussed. Simulations in PROII were completed to supplement SuperPro data from the previous reports. All supporting figures and calculations are located in the Appendix.

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Production of 80,000 Mt/year of 99.9 weight% Cumene

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Allocation of Responsibilities

Jose Garcia-Torres	Group leader, BFD, PFD, Energy balances, Health, Safety, and Hazard Assessments, Environmental Impacts, Discussion of Results
Jose Benitez Ponce	PFD Simulation, Mass balances, Energy balances, Alternative Process Simulation, Profitability, Discussion of Results
Joshua Tai	Equipment sizing, Stream Tables, Equipment Cost, CFDs & Profitability
Jacob Hatt	PFD, Process Description, Health, Safety, and Hazard Assessments, Environmental Impacts, Bare Module Cost, Cost of Utilities, Conclusion
Selena Crawford	Introduction, Previous Works, Health, Safety, and Hazard Assessments, Global, Political, Social, and Environmental Impacts, Conclusion
Giovanna Panelli	Letter of transmittal, Executive summary, Mass balances, Nomenclature, Equipment Descriptions, Conclusion

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Executive Summary

The production of cumene is an essential pathway to producing other chemicals, such as acetone and phenol. Because of its importance as an intermediate product before further processing, processes that optimize the quantity of its production to the cost of raw materials and the construction of the plant would maximize profits. Currently there exists many solutions to the production of cumene at high quantities. However, many such studies do not have adequate optimization, instead often requiring greater feed of raw materials. A proposed process will minimize the required feed of raw materials and produce no less than 80,000 MT/yr of cumene at a purity of 99.9%.

The proposed process is expected to require less capital, since it utilizes the heat generated by the reaction in the reactor to heat the feed stream to the reactor. In addition, due to the added recycle benzene stream, one of the required components in the generation of cumene, less raw materials are required. Thus, the costs are expected to be minimized within the process. The generation of a byproduct in the reactor is minimized to maximize the generation of cumene as a result of the tuned recycle stream. Alternative processes and attempted further optimization have been shown to require more benzene than in the optimal process, but require less capital.

It is expected that the fixed capital investment of the plant would amount to $8.2 million, with a payback period of 1.28 years. With the cost of manufacturing found to be $121.38 million, and the sale of cumene each year to be $132.27 million, a net profit over the lifetime of the plant amounts to $29.29 million. These profits are based on the operating lifetime of 10 years, with 8,000 operating hours per year.

Based on the profitability, recommendations can be made to increase the profits, including careful planning and construction of the proposed process during times when the cost of raw materials is expected to be reasonably low during the operating lifetime of the plant. Since the price of cumene is volatile, a more detailed market analysis would better help with considerations for this recommendation. Other considerations include the construction of an additional plant for direct synthesis of more useful products, such as acetone and phenol, in times when the profitability of cumene is expected to be low. However, similar to the first recommendation, a market analysis on the prices of these two products is encouraged to determine the cost-benefit analysis for the potential of this consideration.

Introduction

Isopropylbenzene, also known as cumene, is a top commodity chemical due to its high demand in various chemical processes. Cumene plays a minor role in gasoline blending, the production of styrene, α-methylstyrene, acetophenone, detergents, di-isopropylbenzene (p-DIBP), etc.; however, the primary use of cumene is as an intermediate in the production of phenol and acetone [1]. In this report we aim to design a process that produces 80,000 Mt/y of 99.9% cumene.

Cumene is manufactured from benzene and propylene, see Eq. 1. A common issue that can occur during production is the undesired side reaction of propylene and cumene to produce p-DIBP, see Eq. 4. p-DIBP is a chemical of little value and therefore it is important to keep the selectivity of this reaction low. Since higher temperatures favor the formation of the byproduct, p-DIBP, it is crucial that lower reactor temperatures are maintained in order to increase the selectivity of cumene. The solid phosphoric acid (SPA) catalyst increases the selectivity of cumene and helps reduce the formation of any unwanted byproducts. The reaction kinetics provided for each reaction are specific to this catalyst.

$$C_3H_6 + C_6H_6 \rightarrow C_9H_{12} \tag{1}$$

$$r_1 = k_1 C_B C_P \tag{2}$$

$$k_1 = 2.80 \text{ x } 10^7 \exp(-104181/RT) \tag{3}$$

$$C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18} \tag{4}$$

$$r_2 = k_2 C_P C_C \tag{5}$$

$$k_2 = 2.32 \text{ x } 10^9 \exp(-146774/RT) \tag{6}$$

Where the units of activation energy are kJ $kmol^{-1}$, R is the ideal gas constant of 8.316 kJ $kmol^{-1}$ K^{-1}, concentrations (C_B, C_P, C_C) are in kmol m^{-3}, the rate of reaction (r_1, r_2) are in kmol m^{-3} s^{-1}, and the temperature (T) is in units of K. The reaction kinetics are based on a SPA catalyst with a void fraction of 0.5 and a density of 2000 kg/m^3 [6].

There are a number of different processes to produce cumene in published literature. In this report, three methods of production have been compared through preliminary economic analyses in an effort to find the most economical and efficient way of manufacturing cumene.

Previous Works

When it comes to designing a chemical process, there are many different ways to approach the matter. After thorough analysis of previous research and literature, the combination of benzene and propene appears to be the most effective way of producing cumene.

Both of the reactions shown in Eq. 1 and in Eq. 4 are exothermic and irreversible. The activation energy (E_A) required for the formation of cumene is 104,174 kJ/kmol, while the activation energy required to produce p-DIBP is 146,742 kJ/kmol. This indicates that there is more of a likelihood for p-DIBP to form at higher temperatures and cumene is more likely to form at lower temperatures. This was an important factor kept in mind while designing the process that maximized the production of cumene.

Sharma et al. proposed that an excess of benzene should be sustained to minimize the formation of p-DIBP during a study of a cumene plant with 300,000 metric tons per annum capacity that used pure benzene and propene with 5 mol% propane impurity as a feed. In this study, the cumene reactor was operated at high temperatures and utilized a trans-alkylator to convert p-DIBP into cumene. It was found that the use of a trans-alkylator had little impact on the project costs and did not heavily impact the design optimization [2].

Pathak et al. used a similar approach to Sharma et al. but suggested replacing the flash tank in the conventional design, with a purge column to reduce the loss of reactants and product. In this design a trans-alkylator was also used in order to convert any unwanted p-DIBP into cumene [3]. This drastically reduced waste and lowered process costs.

Luyben found a way to improve the conventional cumene design process and increase the conversion of propene [4]. The proposed design of Luyben's process produced 88,480 metric tons of cumene per annum using benzene and propylene in a high temperature, high pressure gas phase reactor. With the use of a catalyst, larger reactors, and the heat of the reaction—in order to generate steam—Luyben optimized his design economically. His suggested process resulted in 99% conversion of propene [5].

An alternative process that was considered during the drafting of the final design was a technique that relied on a singular column for distillation, modified from a process illustrated in Flegiel et. al [4]. This process required an increased input of benzene at lower reactor temperatures in order to minimize p-DIBP conversion. The use of extra benzene adds on approximately $6.5 million dollars to raw material costs. Although this process accomplishes the objective of producing 80,000 Mt/y of 99.9% cumene, when held in comparison to the process analyzed in this report, it is significantly more costly and less profitable.

One other alternative process was published by Turton et. al [15], which is often used as a baseline for comparing other chemical processes for the production of cumene from the same reactant. As it is a baseline process, other more optimized processes are preferred, such as those proposed by Sharma et. al and Luyben. The lack of heat integration in this process, in particular from the leaving product stream from the reactor has made the process less efficient and more economically costly than processes that incorporate this technology, as a fired heater is used in place to raise the temperature of the feed stream acceptable for reaction in the plug flow reactor.

The study that much of this report will be based on was one performed by Santos et al. which analyzed what cumene production process is most economically and environmentally efficient. In this process, cumene is created under high temperature, high pressure conditions in a gas-phase packed bed reactor equipped with an acid catalyst. The most effective technology used was a two-flash vessel system to improve energy efficiency and reduce loss of material—which directly resulted in the higher conversion of propylene [6]. This process involves the use of two distillation columns and less benzene input, as opposed to the process mentioned prior that utilized one distillation column and increased benzene input.

Results

The first step in the development of the process was the BFD in Figure 1. The final PFD, Figure 2, was updated according to the equipment used in the PRO/II simulation, which was ultimately informed by preliminary drafts of the PFD and the works of Santos et al. [6].

Process Description

The PFD for the optimal cumene production process is given in Figure 2. The reactants were fed from their storage tanks by pumps P-101 and P-102. Benzene mixed with the recycle in Stream 3 and continued on to mix with propylene before the stream entered a feed effluent heat exchanger (FEHE), E-101. Here, they vaporized and heated up to 142°C. The PFR reactor carried out the conversion of the reactants into cumene and undesired byproduct p-DIBP at 250°C. Excess benzene existed and temperature was held under p-DIBP's heat of formation to prevent the secondary reaction from occurring. Since both reactions were exothermic, boiler feed water entered the reactor to provide cooling and exited as high-pressure steam. Then, the product stream heated up the incoming reactants to R-101 in the FEHE. From there, Stream 8 was sent to the two flash tanks, V-101 and V-102, where most of the propane was removed from the process. Streams 13 and 14 mixed before entering the first distillation tower, T-101, separating benzene, and recycling it back to Stream 2 through pump P-103. The bottoms mixture continued to the second distillation tower, T-102, to separate the cumene from the byproducts. The distillate passed through a cooler and the outcome was a final product of 99.9 wt% cumene.

Block Flow Diagram:

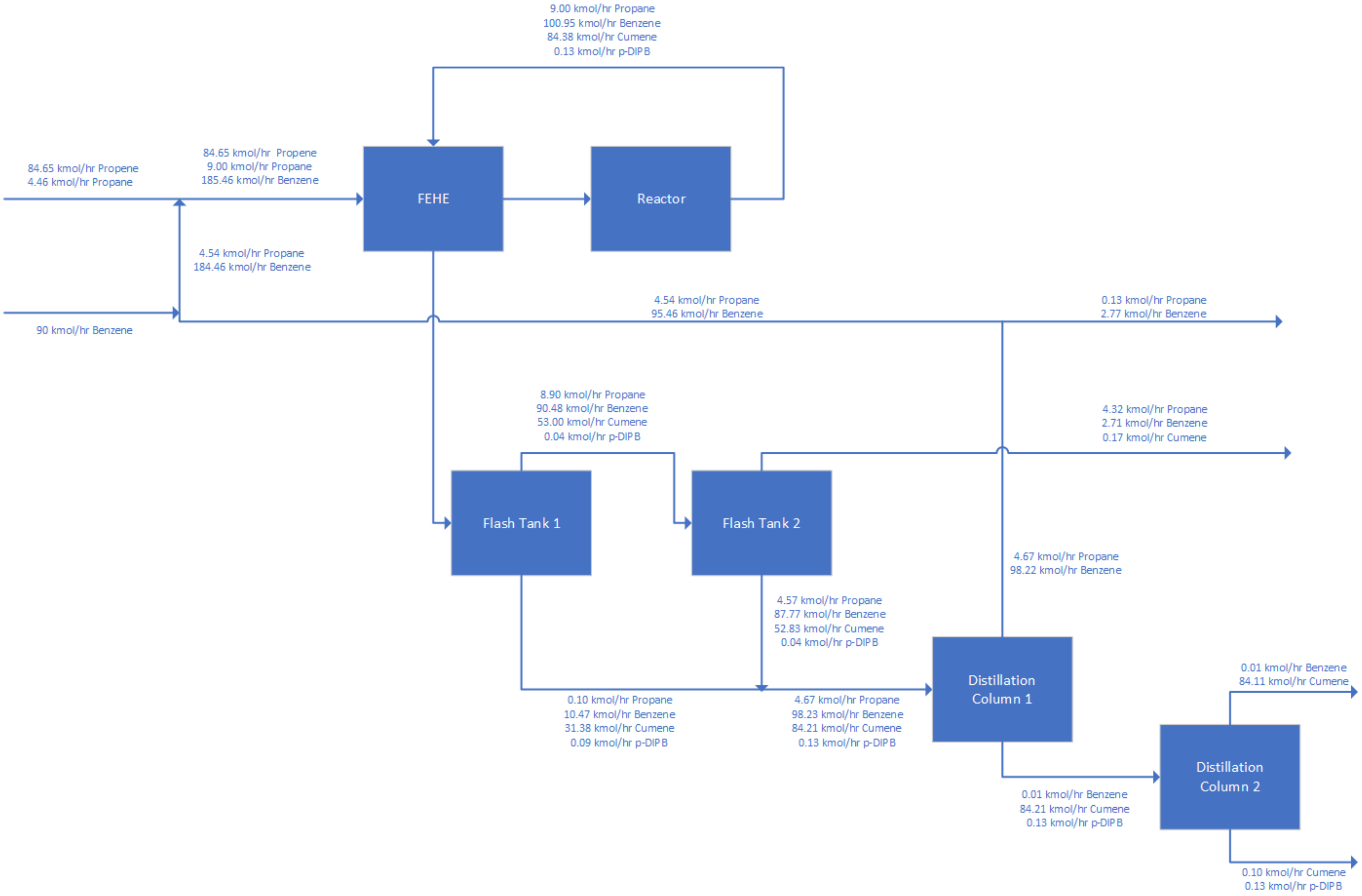


Figure 1. BFD for chosen process with component flow rates (kmol/hr).

Process Flow Diagram

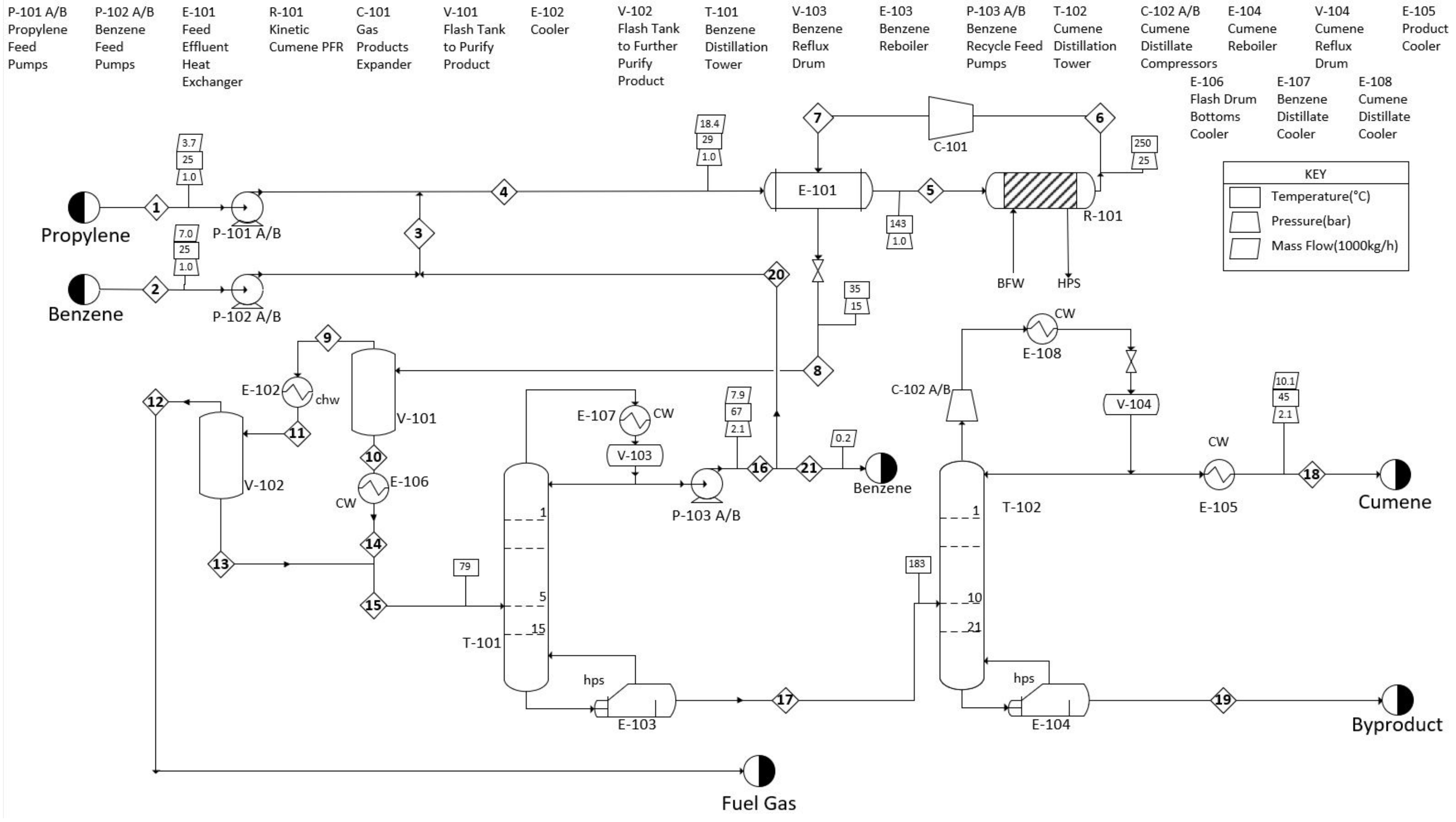
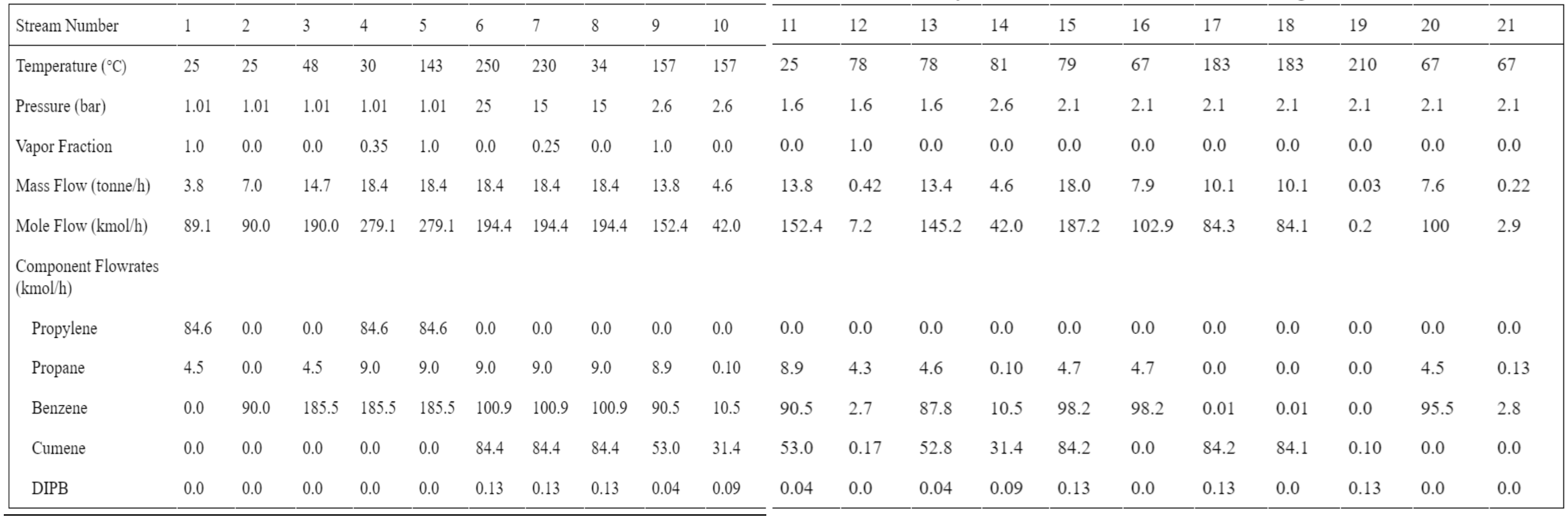


Figure 2. PFD for a process that produces 80,000 Mt/y of 99.9 wt% cumene.

Table 1. Flow Summary Table for Streams 1 to 21 for the Cumene Process Shown in Figure 2



Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Temperature (°C)	25	25	48	30	143	250	230	34	157	157	25	78	78	81	79	67	183	183	210	67	67
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	25	15	15	2.6	2.6	1.6	1.6	1.6	2.6	2.1	2.1	2.1	2.1	2.1	2.1	2.1
Vapor Fraction	1.0	0.0	0.0	0.35	1.0	0.0	0.25	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Flow (tonne/h)	3.8	7.0	14.7	18.4	18.4	18.4	18.4	18.4	13.8	4.6	13.8	0.42	13.4	4.6	18.0	7.9	10.1	10.1	0.03	7.6	0.22
Mole Flow (kmol/h)	89.1	90.0	190.0	279.1	279.1	194.4	194.4	194.4	152.4	42.0	152.4	7.2	145.2	42.0	187.2	102.9	84.3	84.1	0.2	100	2.9
Component Flowrates (kmol/h)																					
Propylene	84.6	0.0	0.0	84.6	84.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Propane	4.5	0.0	4.5	9.0	9.0	9.0	9.0	9.0	8.9	0.10	8.9	4.3	4.6	0.10	4.7	4.7	0.0	0.0	0.0	4.5	0.13
Benzene	0.0	90.0	185.5	185.5	185.5	100.9	100.9	100.9	90.5	10.5	90.5	2.7	87.8	10.5	98.2	98.2	0.01	0.01	0.0	95.5	2.8
Cumene	0.0	0.0	0.0	0.0	0.0	84.4	84.4	84.4	53.0	31.4	53.0	0.17	52.8	31.4	84.2	0.0	84.2	84.1	0.10	0.0	0.0
DIPB	0.0	0.0	0.0	0.0	0.0	0.13	0.13	0.13	0.04	0.09	0.04	0.0	0.04	0.09	0.13	0.0	0.13	0.0	0.13	0.0	0.0

Material Balances

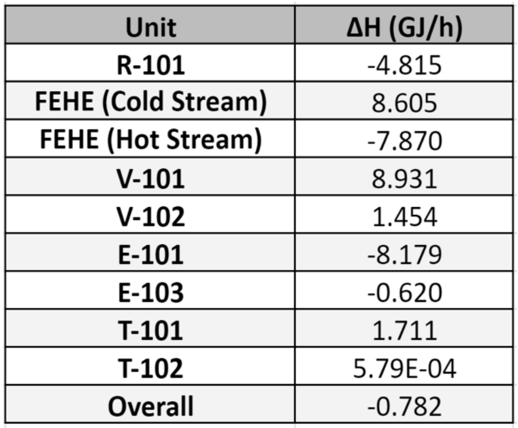
The total hourly amount of cumene produced is 10,109.52 kg. Based on 8000 operating hours/year, this process will produce 80876.16 Mt cumene per year.

Single pass conversion of benzene is 45.57% while propylene is 99.99%. This is as expected due to the large excess of benzene fed into the reactor. Single pass conversion of benzene on the PROII simulation is 45.56%, meaning that there is very small error in the calculations. The overall conversion of benzene was 93.90%, leaving 428.76 kg benzene/h unused throughout the entire process. The purity of the cumene product in stream 18 was 99.99 wt%. Stream 19 contained 64 wt% p-DIBP and 35 wt% cumene. The amount of p-DIBP produced yearly was 171 Mt per year.

Energy Balances

The approach taken to solve the manual energy balances consisted of calculating the change in enthalpy using heats of formation and sensible heat for each chemical species. This calculation was accomplished across major equipment in the process plant. The thermodynamic data for the chemical species present in the process was retrieved from Perry's Handbook (8th Ed.) and the National Institute of Standards and Technology database [16, 20]. Here, heats of formations for the species in both gas and liquid phases were found and incorporated into the calculations. In Perry's Table 2-156, heat capacities were approximated using the hyperbolic function A.1 in the appendix. Extensive description of unit calculations of enthalpy changes are delineated in Appendix A.

The following table demonstrates the energy balance of the chemical species across all major equipment: heat exchangers, reactor, flash tanks, and distillation columns in units of GJ/hr.



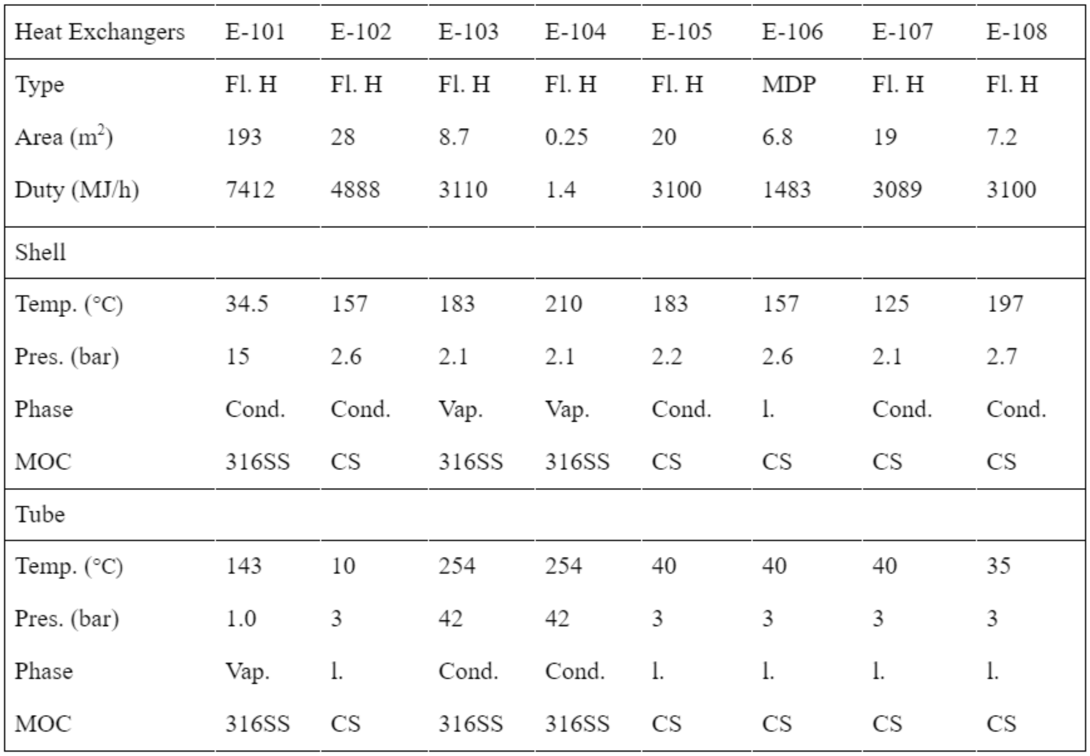
Unit	ΔH (GJ/h)
R-101	-4.815
FEHE (Cold Stream)	8.605
FEHE (Hot Stream)	-7.870
V-101	8.931
V-102	1.454
E-101	-8.179
E-103	-0.620
T-101	1.711
T-102	5.79E-04
Overall	-0.782

Table 2. Enthalpy calculations across major equipment.

*The energy balance is based on the major equipment in the PRO/II simulation

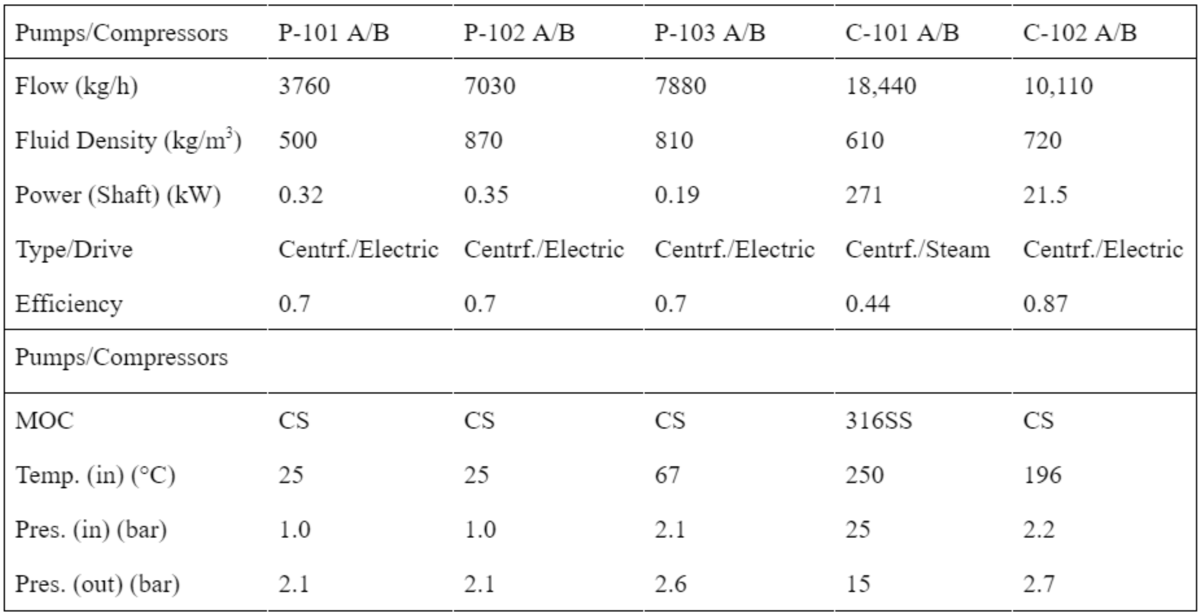
Equipment Sizing, Specifications, and Cost

Table 3. Equipment Sizing and Specifications, Heat Exchangers



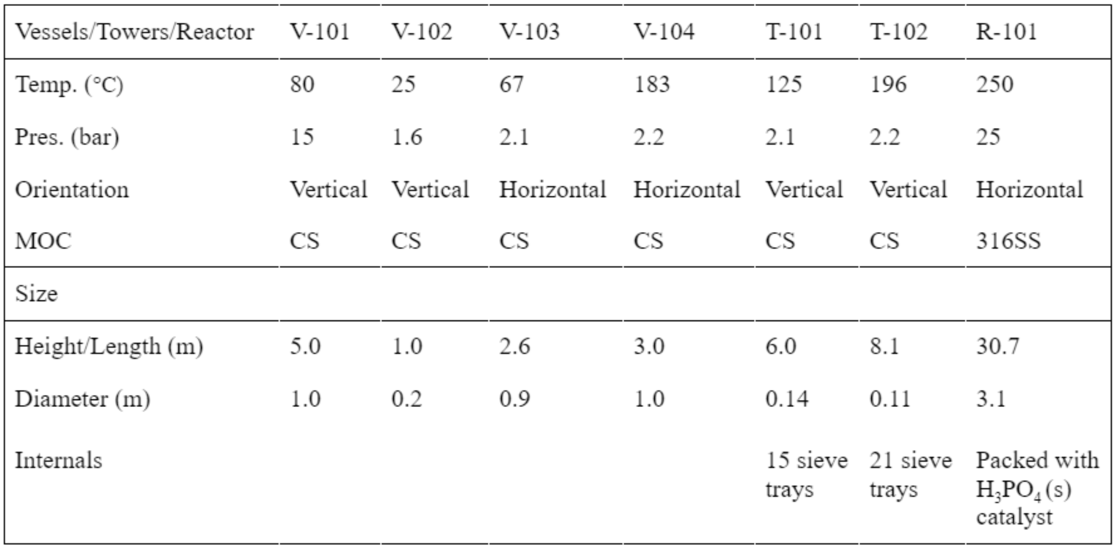
Heat Exchangers	E-101	E-102	E-103	E-104	E-105	E-106	E-107	E-108
Type	Fl. H	Fl. H	Fl. H	Fl. H	Fl. H	MDP	Fl. H	Fl. H
Area (m^2)	193	28	8.7	0.25	20	6.8	19	7.2
Duty (MJ/h)	7412	4888	3110	1.4	3100	1483	3089	3100
Shell								
Temp. (°C)	34.5	157	183	210	183	157	125	197
Pres. (bar)	15	2.6	2.1	2.1	2.2	2.6	2.1	2.7
Phase	Cond.	Cond.	Vap.	Vap.	Cond.	l.	Cond.	Cond.
MOC	316SS	CS	316SS	316SS	CS	CS	CS	CS
Tube								
Temp. (°C)	143	10	254	254	40	40	40	35
Pres. (bar)	1.0	3	42	42	3	3	3	3
Phase	Vap.	l.	Cond.	Cond.	l.	l.	l.	l.
MOC	316SS	CS	316SS	316SS	CS	CS	CS	CS

Table 4. Equipment Sizing and Specifications, Pumps and Compressors



Pumps/Compressors	P-101 A/B	P-102 A/B	P-103 A/B	C-101 A/B	C-102 A/B
Flow (kg/h)	3760	7030	7880	18,440	10,110
Fluid Density (kg/m^3)	500	870	810	610	720
Power (Shaft) (kW)	0.32	0.35	0.19	271	21.5
Type/Drive	Centrf./Electric	Centrf./Electric	Centrf./Electric	Centrf./Steam	Centrf./Electric
Efficiency	0.7	0.7	0.7	0.44	0.87
Pumps/Compressors					
MOC	CS	CS	CS	316SS	CS
Temp. (in) (°C)	25	25	67	250	196
Pres. (in) (bar)	1.0	1.0	2.1	25	2.2
Pres. (out) (bar)	2.1	2.1	2.6	15	2.7

Table 5. Equipment Sizing and Specifications, Vessels, Towers, and PFR



Vessels/Towers/Reactor	V-101	V-102	V-103	V-104	T-101	T-102	R-101
Temp. (°C)	80	25	67	183	125	196	250
Pres. (bar)	15	1.6	2.1	2.2	2.1	2.2	25
Orientation	Vertical	Vertical	Horizontal	Horizontal	Vertical	Vertical	Horizontal
MOC	CS	CS	CS	CS	CS	CS	316SS
Size							
Height/Length (m)	5.0	1.0	2.6	3.0	6.0	8.1	30.7
Diameter (m)	1.0	0.2	0.9	1.0	0.14	0.11	3.1
Internals					15 sieve trays	21 sieve trays	Packed with H_3PO_4 (s) catalyst

Tables 3, 4, and 5 present the equipment sizing and specifications for the heat exchangers, pumps/compressors, and vessels/towers/reactor, respectively. The equipment sizing was calculated using heuristic equations and relations, demonstrated in Appendix A.

The equipment costs, or bare module costs, are presented in Table A.27 in the appendix. The bare module cost of all the equipment involved in the process was $6,934,300. The bare module costs for the compressors and vessels were $2,298,800 and $2,070,700, respectively, which made up for more than half of the total bare module cost. The equipment with the lowest bare module cost were the pumps at $89,700. This was expected because the pumps had low shaft power and were used to transport liquid. The plug-flow reactor alone had a bare module cost of $1,160,000. Also, the bare module costs for the 8 heat exchangers and 2 distillation columns were $1,047,300 and $267,800, respectively.

Process Economics and Profitability

The raw materials involved in this process are benzene, propylene, propane, and SPA as the catalyst. The market prices of these raw materials were retrieved from Echemi.com [21-24]. From this source, an average market price was calculated from months March through May of 2021. The average of these market prices is summarized in Table A.24. The raw materials prices originate from a supplier in China, which was one of the cheapest suppliers. These prices were found in the Chinese currency of Yuan per metric ton and were converted to USD per metric ton (1 USD = 6.42 Yuan). The amounts of each of these raw materials were calculated from kilomole per hour to metric ton to year to allow a facilitated calculation to the yearly total cost of raw materials. The amount of SPA required was calculated using the density of the SPA catalyst (2000 kg/m^3) and the volume of the tubular reactor according to Pro/II (~480 m^3). The total raw material cost based on the main process was \$95.10 million, which was a moderate amount considering that the market prices of these raw materials were very volatile.

The fixed capital cost (FCI) was determined by calculating the total module cost (C_{TM}) from the bare module cost (C_{BM}) using Equation 7. The C_{BM} of all the equipment involved in the process

$$C_{TM} = 1.18 \int_{i=1}^{n} C_{BM,i} \tag{7}$$

was \$6,934,300, derived from equations in Turton Appendix A, and using the program CAPCOST. This resulted in a C_{TM} of \$8,182,474. The FCI was divided evenly into years 1 and 2 of the plant construction. According to the problem statement, the cost of land and salvage value were 10% of the FCI, or \$818,247.40. Working capital was assumed to be 20% of the FCI, or \$1,636,494.80. These cash flows were integrated into the profitability criteria according to Turton. The non-discounted and discounted cash flows are summarized in Tables A.25 and A.26, respectively. From the calculated profitability criteria, non-discounted and discounted cumulative cash flow diagrams were created (Figure 3 and 4). The profitability metrics were calculated and are summarized in Tables 7 and 8. Calculations related to the profitability criteria and metrics can be found in Appendix A.

The profitability criteria of this process are shown below:

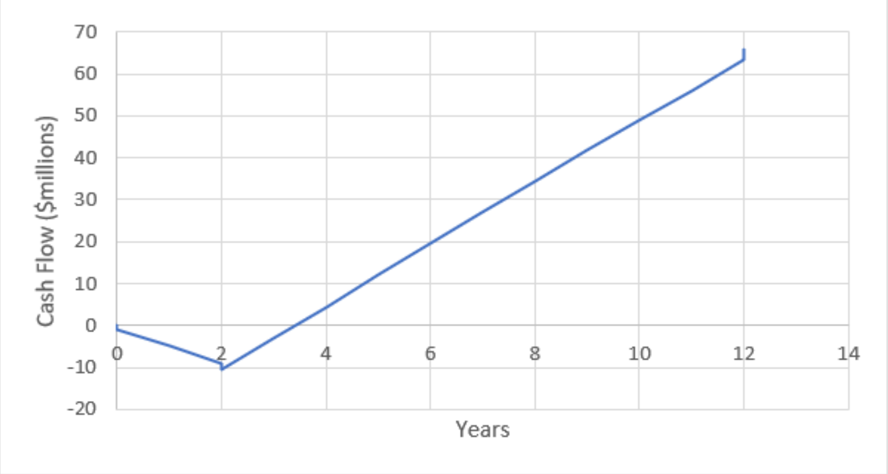


Figure 3. Non-discounted cumulative cash flow diagram.

Table 6. Profitability Metrics from the Non-discounted Cumulative CFD

Non-discounted Profitability Metrics	
Cumulative Cash Position ($M)	65.94
Cumulative Cash Ratio	7.20
Payback Period (Years)	1.09
Rate of Return on Investment (%)	80.58

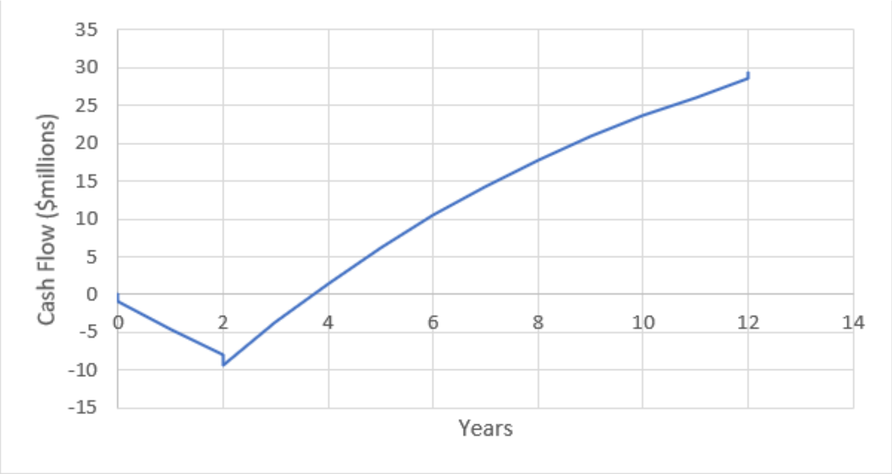


Figure 4. Discounted cumulative cash flow diagram

Table 7. Profitability Metrics from the Discounted Cumulative CFD

Discounted Profitability Criteria	
Net Present Value ($M)	29.29
Present Value Ratio	4.16
Discounted Payback Period (yr)	1.28

The revenue of the process consisted of cumene sales and the fuel credit of p-DIPB mixed with cumene. Junqueira et al. provided an optimal cumene sell price of $198.73/kmol, which is equivalent to $1,653.41/Mt [6]. Since a minimum of 80,000 Mt/year is produced, the profit of cumene sales alone is $132.27 million per year. The bottoms of the second distillation column consists of 0.10 kmol/hr cumene and 0.13 kmol/hr p-DIPB. The standard heats of combustion for p-DIBP and cumene are 6.82 GJ/kmol and 5.00 GJ/kmol, respectively. The fuel credit value is $3.16/GJ [15]. In an 8,000-hr operating year, $35,053 is obtained as fuel credit per year, which was accounted for as an extra source of revenue per year.

The cost of manufacture (COM_d) was calculated using the cost of labor (C_{OL}), the cost of utilities (C_{UT}), the fixed capital investment (FCI_L), and the cost of raw materials. For the process, 14 operators are required and are paid $66,910 per year for a total cost of labor of $936,700 per year. The cost of utilities was calculated from the equipment duties and summed up to $307,000/year. As mentioned previously, the FCI was made equal to the total module cost, which was calculated to be $8,182,474. The waste treatment cost of the process was not considered in this process design due to variations in price according to region. Lastly, the cost of raw materials summed up to be $95.10 million, as stated previously. Overall, the cost of manufacture of this process was calculated to be $121.38 million. The details of this calculation are demonstrated in Appendix A.

Discussion

Screening for the Optimal Process

An ideal process that would be best for the production of cumene will optimize for the cost of units/capital investment and the raw materials needed to produce the required 99.9 wt% 80,000 MT/yr cumene. A common process referenced in literature [15], is often used as the baseline point of reference for more robust and optimized processes. Summarized in Appendix A.30 - A.32, preliminary screening in the SuperPro simulation software demonstrated higher purchase costs and raw materials usage of the process illustrated by Turton.

A comparison of the equipment costs and the cost of raw materials between the two processes clearly outline the motive behind the decision to move forward with the optimized process for further simulation. The raw materials are the largest contributor to the yearly cost of manufacturing. The process proposed by Turton is forgone, as the optimized process is less costly than the alternative.

Ongoing simulation and studying of the ideal process involved further optimization, adding or removing equipment that may have had only a minor impact on the generation of cumene. Although such optimizations were attempted, no such equipment could have been removed that would have impacted the economics of the process positively. Removing the second distillation column (T-102) was proven to be a more expensive process, requiring more benzene feed. While removing the pump (P-103) after the first distillation column would have not properly transported the recycle stream with sufficient pressure.

Assumptions, Limitations

Various assumptions for the outlined cumene production process were made for successful simulation. Limitations were identified in SuperPro, which limited the reproduction of the simulation as outlined by Fleigel, et al [4], including the lack of a unit for gas expansion after leaving the PFR, and the ability to modify the distillation column T-102 to include a compressor following the leaving vapor stream shortly before entering the condenser. The first issue was addressed by substituting the compressor for the gate valve, the compressor being C-101A/B. The second was assumed to not contribute significantly to the total energy requirements, relative to those from the distillation column, the PFR and the heat exchanger.

Other assumptions made included the lack of leaks in the process, which would otherwise reduce the amount of cumene generated, and include additional mass balances from these leaks, and that the only reactions occurring in the PFR include only the production of cumene and p-DIBP. A source of error with regards to the energy balance is likely for the operation of the gate valve and the absence of the compressor, but it is not anticipated that the material balances would be affected.

Methodology of Results Collection and Discussion

The results for the production process of 80,000 MT/yr cumene were obtained through PRO/II Process Engineering simulation software. The continuous process was simulated on an hourly basis with propylene and benzene feeds of 89.1 kmol/h and 90 kmol/h, respectively. Before entering the reactor, benzene was 119.1% in excess in respect to propylene and the inlet stream was raised to a temperature of 143 °C from a feed effluent heat exchanger, giving preference to the generation of cumene over p-DIBP. The pressure within the kinetic tubular reactor was set to 25 bar with no pressure drop to ensure effective mass transfer of the reactants to the SPA catalyst surface. Ultimately, cumene exited the process via the second distillation column with 20 trays at 84.11 kmol per hour and 99.99% purity for a simulated production of 80,877 metric tons per 8000-hour year.

Stemming from the sizing of the equipment, and the work from Santos et al [6], the resulting stream tables and mass balances were completed after completing the PRO/II simulation, when the reports of the streams via stream tables were compiled. After sizing was completed per the heuristics outlined in Appendix A, the bare module cost was calculated, which informed the economics of the construction of the plant, determining the profitability and the payback period of the fixed capital.

The conversion of benzene overall was less than ideal (< 95-99%). This could have been preferably increased; however, the presence of a leaving stream shortly after the first distillation column indicates a decreased benzene stream entering in through the recycle. If the benzene stream were to increase through the recycle, a larger proportion of this component would have been consumed, as the kinetics of cumene generation depend on benzene concentration. The presence of a leaving stream after going through a splitter was necessary to allow simulation through PRO/II, which would have otherwise not have allowed complete simulation by convergence of the numerical methods used in the software. Perhaps more robust simulation software would have avoided this caveat, and would have indicated an increase in benzene conversion. The loss of benzene contributes to the increase in raw materials cost, as it is treated as a waste stream with loss in potential cumene generation.

Health, Safety, and Hazard Assessments

Health and fire hazards, exposure limits and explosive limits of the five chemicals are summarized in Appendix C (Tables C.1 - C.3). Most important to note are the consequences of benzene mishandling or leaks, which presents a danger to health, due to the low PEL, REL and TLV, and the wide range of effects, ranging from simple dizziness to more dire cases involving coma or even death [7]. Since benzene is used in large amounts in the preferred process, special care must be taken to ensure minimal exposure to the chemical.

No information for exposure limits has been found for p-DIBP, though there exists a measurable concern for the health effects from exposure to this chemical [8]. However, very little p-DIBP is produced in the preferred process, and is thus a minor concern.

Global, Political, Social, and Environmental Impacts

Due to its various uses, there is a large global demand for cumene. The chemical is among the world's top large-scale productions alongside benzene, ethylbenzene, ethylene, and propylene [1]. In 2016 the Global Cumene Market was valued at $18.8 billion USD and this figure is expected to steadily grow due to the increasing demand for the chemical [9]. The global demand for cumene is estimated to have grown from 12.4 million metric tons to 18 million metric tons over the course of only 9 years [4].

Biochemical and environmental data is summarized in Appendix C (Table C.4), describing properties of bioaccumulation in the environment and in animals and plants. Benzene presents a measurable danger to life, as it produces acute toxicity causing shortened life spans and other life altering effects to aquatic organisms, should it be released to the environment. Benzene can also destroy agricultural crops, causing death to plants and roots. Otherwise, this chemical may break down into photochemical smog, if it does not interact with life [10]. Other chemicals involved in the preferred process breakdown quickly and do not pose a measurable threat to life and the environment, should leaks occur [11-14].

Conclusions and Recommendations

Upon the completion of the proposed simulation, it was found that this simulation produced less waste than the process presented in Turton. This was due to Turton's process forming more p-DIBP in the reactor and excess benzene that did not react or recycle. The process utilizing one distillation tower is also not recommended since it required around $6.5 million more benzene than the chosen process.

Cumene production is favored at lower reactor temperatures with an excess of benzene in the feed. By incorporating these concepts into the design, 99.99% propylene conversion and 93.9% overall conversion of benzene was achieved, with only an error of 0.02% in the mass balance calculation.

With a fixed capital investment of $8.182 million, the discounted payback period for this process is 1.28 years. The profit from selling the finished product is estimated to be $132.27 million per year. After considering the cost of manufacturing and other expenses, the NPV after 10 years of operation amounts to $29.29 million, concluding this process is highly profitable and suggested.

Since all chemicals pose a threat to health, do not exceed the TLV, especially for benzene and cumene. Due to all of the chemicals' flammable nature, explosions can occur. It is highly advisable to add controllers to the reactor, to ensure operation remains below hazardous temperature and pressure limits. The proposed process produces no identified groundwater or air emissions, meaning that no environmental impact is made due to pollution.

It is recommended that the plant be built during periods of low price for raw materials since they represent a majority of the cost. Since cumene has fluctuating market prices, it is suggested to operate the plant during periods of high demand to maximize profit. If it is unlikely cumene market prices will increase during the life of manufacturing, consider adding another process in the current plant or a nearby one to convert the product into other chemicals to maximize profitability.

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Nomenclature

Symbol	**Description**
BFW	Boiler feed water
C_B	Concentration of Benzene (kmol/m^3)
C_{BM}	Bare module cost
C_C	Concentration of Cumene (kmol/m^3)
C_P	Concentration of Propylene (kmol/m^3)
C_p	Specific heat capacity (J/kmol-K)
C^o_p	Purchase cost of equipment
C_{OP}	Cost of operating labor
C_{TM}	Total module cost
C_{UT}	Cost of utilities
COM_D	Cost of manufacturing
chw	Chilled water
cw	Cooled water
p-DIBP	para di-isopropylbenzene, undesired product
e	Efficiency of pumps
F	Flow rate or shape factor
F_{BM}	Bare module factor
F_M	Material Factor
F_P	Pressure Factor
FCI	Fixed Capital Investment

FEHE	Feed Effluent Heat Exchanger
ΔH	Enthalpy (GJ/kmol, kJ/kmol)
ΔH_f^0	Heat of formation (GJ/kmol, kJ/kmol)
ΔH_i	Enthalpy for species *i* (GJ/kmol, kJ/kmol)
hps	High pressure steam
i	Species
k_1	Reaction rate constant of Cumene reaction
k_2	Reaction rate constant of p-DIBP reaction
λ	Enthalpy of vaporization (kJ/mol)
m	Mass flow rate (kg/h)
MOC	Material of construction
n	Number of moles (kmol, mol)
Q	Heat (GJ/kmol, kJ/kmol)
R	Gas constant (8.316 kJ/kmol·K)
R/R_{min}	Reflux ratio
r_1	Reaction rate of cumene reaction (kmol/m^3s)
r_2	Reaction rate of p-DIBP reaction (kmol/m^3s)
SPA	Solid phosphoric acid
T	Temperature (K, °C)
ΔT	Change in temperature (K, °C)
T_0	Initial temperature (K, °C)
ΔT_{lm}	Log mean temperature difference (K, °C)

u	Gas velocity (m/s)
W_s	Shaft power (kW)
x_{dr}(%)	Efficiency of compressor
z_1	Compressibility factor

Appendices

Appendix A. Sample Calculations

<u>Material Balances</u>

Reactor single pass conversion: 45.56% Benzene

Table A.1 Molar balance calculations (kmol/h)

Species	S1 (IN)	S2 (IN)	S3	S4	S5
PROPENE	84.65	0.00	0.00	84.65	84.65
PROPANE	4.46	0.00	4.54	9.00	9.00
BENZENE	0.00	90.00	185.46	185.46	185.46
CUMENE	0.00	0.00	0.00	0.00	0.00
PDIPBN	0.00	0.00	0.00	0.00	0.00
Total (kmol)	89.10	90.00	190.00	279.10	279.10

Species	S6	S7	S8	S9	S10
PROPENE	0.00	0.00	0.00	0.00	0.00
PROPANE	9.00	9.00	9.00	8.90	0.10
BENZENE	100.95	100.95	100.95	90.48	10.47
CUMENE	84.38	84.378	84.38	53.00	31.38
PDIPBN	0.13	0.133	0.13	0.04	0.09
Total (kmol)	194.46	194.46	194.46	152.42	42.04

Species	S11	S12 (OUT)	S13	S14	S15
PROPENE	0.00	0.00	0.00	0.00	0.00
PROPANE	8.90	4.32	4.57	0.10	4.67
BENZENE	90.48	2.71	87.77	10.47	98.23
CUMENE	53.00	0.17	52.83	31.38	84.21
PDIPBN	0.04	0.00	0.04	0.09	0.13
Total (kmol)	152.42	7.21	145.21	42.04	187.25

S16	S17	S18 (OUT)	S19 (OUT)	S20	S21 (OUT)
0.00	0.00	0.00	0.00	0.00	0.00
4.67	0.00	0.00	0.00	4.54	0.13
98.22	0.01	0.01	0.00	95.46	2.77
0.00	84.21	84.11	0.10	0.00	0.000
0.00	0.13	0.00	0.13	0.00	0.00
102.90	84.35	84.12	0.23	100.00	2.90

Table A.2 Mass Balance calculations (kg/h)

Species	S1 (IN)	S2 (IN)	S3	S4	S5
PROPENE	3561.86	0.00	0.00	3561.86	3561.86
PROPANE	196.45	0.00	200.30	396.75	396.75
BENZENE	0.00	7030.26	14486.83	14486.83	14486.83
CUMENE	0.00	0.00	0.00	0.00	0.00
PDIPBN	0.00	0.00	0.00	0.00	0.00
Total (kg)	3758.31	7030.26	14687.13	18445.44	18445.44

Species	S6	S7	S8	S9	S10
PROPENE	0.02	0.02	0.02	0.02	0.00
PROPANE	396.75	396.75	396.75	392.34	4.41
BENZENE	7885.32	7885.32	7885.32	7067.85	817.47
CUMENE	10141.70	10141.70	10141.70	6370.20	3771.49
PDIPBN	21.65	21.65	21.65	6.44	15.20
Total (kg)	18445.44	18445.44	18445.44	13836.86	4608.58

Species	S11	S12 (OUT)	S13	S14	S15
PROPENE	0.02	0.02	0.00	0.00	0.00
PROPANE	392.34	190.65	201.69	4.41	206.10
BENZENE	7067.85	212.00	6855.85	817.47	7673.32
CUMENE	6370.20	20.22	6349.99	3771.49	10121.48
PDIPBN	6.44	0.00	6.44	15.20	21.65
Total (kg)	13836.86	422.88	13413.97	4608.58	18022.55

S16	S17	S18 (OUT)	S19 (OUT)	S20	S21 (OUT)
0.00	0.00	0.00	0.00	0.00	0.00
206.10	0.00	0.00	0.00	200.30	5.80
7672.63	0.69	0.69	0.00	7456.57	216.07
0.01	10121.47	10109.52	11.94	0.00	0.01
0.00	21.65	0.00	21.65	0.00	0.00
7878.75	10143.80	10110.22	33.59	7656.87	221.88

10109.52 kg cumene/h * 8000 hours/year * (1 Mt/1000 kg) = 80876.16 Mt cumene/year

Table A.1 was converted to Table A.2 by multiplying the respective values for each component by their molar weight. The mass balances utilized a calculation with a recycle stream and multiple iterations.

Benzene: (90.0000 kmol/h * 78.114 kg benzene/kmol benzene) = 7030.26 kg benzene/h
Cumene: (84.0946 kmol/h * 120.194 kg cumene/kmol cumene) = 10107.6712 kg cumene/h

Propane: (4.4400 kmol.h * 44.096 kg propane/kmol propane) = 195.7862 kg propane/h
Propylene: (84.3600 kmol/h * 42.08 kg propylene/kmol propylene) = 3549.8688 kg propylene/h
p-DIBP: (0.1175 kmol/h * 162.264 kg p-DIBP/kmol p-DIBP) = 19.0690 kg p-DIBP/h

Single pass benzene calculated as follows:

(185.46 kmol benzene/h - 100.95 kmol benzene/h)/(185.46 kmol benzene/h) = .4556 * 100% = **45.56%**

Overall mass balance:

Mass in = 3758.31 kg/hr + 7030.26 kg/hr = 10788.57 kg/hr (Streams 1 and 2)

Mass out = 422.88 kg/hr + 10110.22 kg/hr + 33.59 kg/hr + 221.88 kg/hr = 10788.57 kg/hr (Streams 12, 18, 19, and 21)

In - Out = 10788.57 kg/hr - 10788.57 kg/hr = **0**

Energy Balances

The coefficients *A*, *B*, *C*, *D*, and *E* are specific to each species and summarized in Table A.3. The specific heat approximation is valid for temperatures ranging from 200 K to 1500K. In this process, the chosen reference point was 25 °C (298.15K) and 1 atm (1.013 bar), where the heat of formations and the sensible heat were approximated. Figure A.1 in the appendix demonstrates the heat capacity and temperature correlation for benzene in the gas phase. The linear fit (orange line) showed that the C_P vs Temperature data is significantly linear with an R^2 value of 99.6%. This linear correlation demonstrated the Trapezoidal Rule was a valid method for approximating the sensible heat of each chemical species using the heat capacities at various temperatures. For the process, the sensible heats were approximated from a temperature range of 298 K to 523 K. Therefore, it was safe to approximate the sensible heat using methods like the Trapezoidal Integration (Eq. A.2). The sensible heat approximation was added to the heat of formation value to obtain the total change in enthalpy for each species, *i* (Eq. A.3). Once each enthalpy was calculated, the total change in enthalpy across the equipment was calculated by Equation A.4.

Since thermodynamic data was limited to values at STP, the main assumptions used in the energy balance were constant pressure of 1 atm and $Q = \Delta H$. Data was retrieved for all species except p-DIBP. Both Perry's Handbook and the NIST contain little to no thermodynamic data for the byproduct. However, DIBP was produced in such a *very* low amount (> 0.0001%) in the reactor that it was considered negligible. Therefore, p-DIBP was omitted from the energy balance calculations. Lastly, energy balances were calculated across all equipment except the mixers, due to little or no significant change in temperature, thus no change in enthalpy.

Table A.3 Heat of formation and specific heat constants of species in gas phase.

Species	H_f (GJ/Kmol*K)	A	B	C	D	E
Benzene (g)	0.08288	44767	230850	1479.2	168360	677.66
Cumene (g)	0.004	108100	379320	1750.5	300270	794.8
Propane (g)	-0.10468	51920	192450	1626.5	116800	723.6
Propylene (g)	0.02023	43852	150600	1398.8	74754	616.46

$$C_p = A + B\left[\frac{C/T}{\sinh C/T}\right] + D\left[\frac{E/T}{\cosh E/T}\right] \tag{A.1}$$

Table A.4 Specific heat values at temperatures utilized in the process.

	Benzene	Cumene	Propane	Propylene
T (K)	**Cp (J/kmol*K)**	**Cp**	**Cp**	**Cp**
284.15	77466.28268	143048.346	70562.52586	62521.48564
298.15	82030.02213	149401.0399	73465.89015	64780.13265
323.25	90199.93828	161341.6824	78767.44755	68781.54252
340	95559.32403	169520.9033	82310.52355	71400.16575
353.3	99728.87705	176048.2631	85100.06207	73445.70722
354.2	100007.8597	176489.6845	85287.70809	73583.0293
373.15	105779.5663	185740.548	89197.29661	76442.52188
400	113597.5982	198577.1637	94575.63563	80395.0373
420	119135.6311	207830.2754	98443.71111	83271.05187
427.2	121069.8736	211085.1522	99806.47445	84293.49541
440	124432.2808	216764.793	102190.5287	86095.42277
451.2	127296.0347	221618.6198	104236.6685	87656.3642
460	129496.1806	225354.8843	105818.8471	88872.96699
480	134339.0508	233590.6789	109334.3466	91607.08532
487.2	136030.8652	236468.8583	110573.647	92581.15262
500	138973.8793	241473.712	112744.0708	94299.71253
518.15	143010.912	248329.909	115753.0184	96707.90138
523	144063.7103	250115.386	116544.0228	97345.69006

$$\int_{T_0}^{T} C_P\,dT = (T - T_0)\cdot\frac{C_P(T) + C_P(T_0)}{2} \tag{A.2}$$

*Trapezoidal Rule Integration equation

$$\Delta H_i = \Delta H_f^o + \int_{T_0}^{T} C_P\,dT \tag{A.3}$$

$$\Delta H = \Sigma n_i \Delta H\ (out) - \Sigma n_i \Delta H_i\ (in) \tag{A.4}$$

Energy Balance Sample Calculation

Reference: C (s), O_2 (g), N_2 (g), H_2 (g) at 25°C, 1 atm

Substance	n_{in} (mol)	$\hat{H}_{in}$ (kJ/mol)	n_{out} (mol)	$\hat{H}_{out}$ (kJ/mol)
C_3H_6	84.65	$\hat{H}_1$	0	$\hat{H}_4$
C_3H_8	9.00	$\hat{H}_2$	9.00	$\hat{H}_5$
C_6H_6	185.46	$\hat{H}_3$	100.95	$\hat{H}_6$
C_9H_{12}	-	-	84.38	$\hat{H}_7$
$C_{12}H_{18}$	-	-	0.13	$\hat{H}_8$ (negligible)

C_3H_6 (142°C): $\hat{H}_1 = (\hat{H}_f^\circ)_{C_3H_6} + \int_{25°C}^{142°C} (C_p)_{C_3H_6} dT$

$= (20.23 + 8.61)$ kJ/mol $= 28.84$ kJ/mol

C_3H_8 (142°C): $\hat{H}_2 = (\hat{H}_f^\circ)_{C_3H_8} + \int_{25°C}^{142°C} (C_p)_{C_3H_8} dT$

$= (-104.68 + 9.99)$ kJ/mol $= -94.69$ kJ/mol

C_6H_6 (142°C): $\hat{H}_3 = (\hat{H}_f^\circ)_{C_6H_6} + \int_{25°C}^{142°C} (C_p)_{C_6H_6} dT$

$= (82.88 + 11.67)$ kJ/mol $= 94.55$ kJ/mol

C_3H_6 (250°C): $\hat{H}_4 = (\hat{H}_f^\circ)_{C_3H_6} + \int_{25°C}^{250°C} (C_p)_{C_3H_6} dT$

$= (20.23 + 18.23)$ kJ/mol $= 38.46$ kJ/mol

C_3H_8 (250°C): $\hat{H}_5 = \left(\hat{H}_f^\circ\right)_{C_3H_8} + \int_{25°C}^{250°C} \left(C_p\right)_{C_3H_8} dT$

$= (-104.68 + 21.36)$ kJ/mol $= -83.32$ kJ/mol

C_6H_6 (250°C): $\hat{H}_6 = (\hat{H}_f^\circ)_{C_6H_6} + \int_{25°C}^{250°C} (C_p)_{C_6H_6} dT$

$= (82.88 + 25.42)$ kJ/mol $= 108.30$ kJ/mol

C_9H_{12} (250°C): $\hat{H}_7 = (\hat{H}_f^\circ)_{C_9H_{12}} + \int_{25°C}^{250°C} (C_p)_{C_9H_{12}} dT$

$= (4.00 + 20.74)$ kJ/mol $= 48.92$ kJ/mol

$C_{12}H_{18}$ (250°C): $\hat{H}_8 = (\hat{H}_f^\circ)_{C_{12}H_{18}} + \int_{25°C}^{250°C} (C_p)_{C_{12}H_{18}} dT$ = not considered

$\Delta H = \Sigma n_i \hat{H}_i\ (out) - \Sigma n_i \hat{H}_i\ (in)$ = [0 mol*(38.46 kJ/mol) + 9.00 mol*(-83.32 kJ/mol) + 100.95 mol*(108.30 kJ/mol) + 84.38 mol*(48.92 kJ/mol)] – [84.65 mol*(28.84 kJ/mol) + 9.00 mol* (-94.69 kJ/mol) + 185.46 mol*(94.55 kJ/mol)] = 14,310.9 kJ – 19,124.1 kJ = **-4,815.1 kJ**

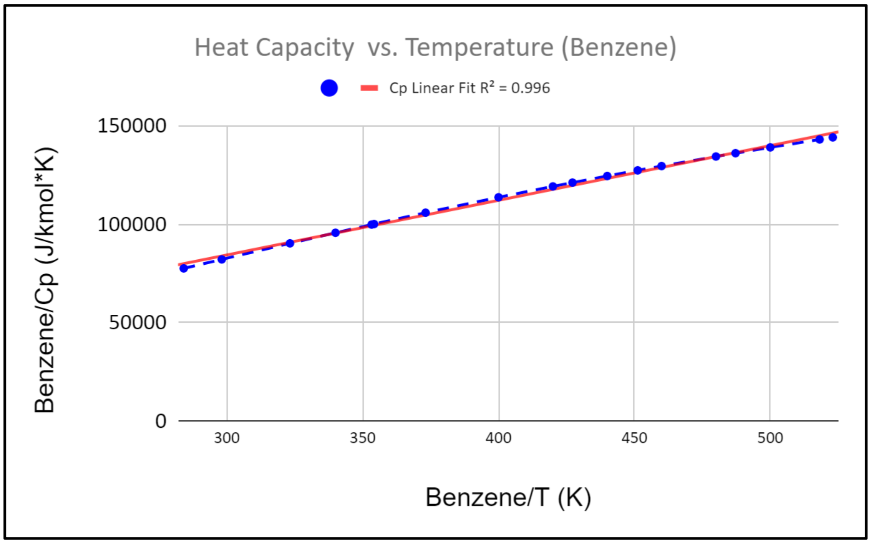

Figure A.1 Heat capacity correlation for Benzene.

*This figure was created to demonstrate that the heat capacity of chemical species like benzene was linear enough to approximate the sensible heat via the Trapezoidal Method.

Table A.5 Energy balance across PFR

Plug Flow Reactor				
Species	**IN (kmol) [S-105]**	**ΔH (kJ/kmol)**	**OUT (kmol) [S-106]**	**ΔH (kJ/kmol)**
PROPENE	84.65	0.0288	0.00	--
PROPANE	9.00	-0.0946	9.00	-0.08331
BENZENE	185.46	0.09458	100.95	0.1083
CUMENE	0.00	--	84.38	0.04891
ΔH (GJ/h)	**-4.8146**			

Table A.6 Energy balance of the cold stream across the heat exchanger (FEHE)

Heat Exchanger (FEHE)					
IN (S-104)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPENE (l)	--	--	--	--	--
PROPENE (g)	20410	64.78013265	65.55923937	298	303

$\Delta H = \Sigma n_i \widehat{H}_i\,(out) - \Sigma n_i \widehat{H}_i\,(in)$ = [0 mol*(38.46 kJ/mol) + 9.00 mol*(-83.32 kJ/mol) + 100.95 mol*(108.30 kJ/mol) + 84.38 mol*(48.92 kJ/mol)] – [84.65 mol*(28.84 kJ/mol) + 9.00 mol* (-94.69 kJ/mol) + 185.46 mol*(94.55 kJ/mol)] = 14,310.9 kJ – 19,124.1 kJ = **-4,815.1 kJ**

PROPANE (l)	-119800	119.6	--	298	303
PROPANE (g)	-104700	73.46589015	74.48409453	298	303
BENZENE (l)	49000	135.69	--	298	303
BENZENE (g)	82900	82.03002213	83.61455743	298	303
OUT (S-105)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPENE (g)	20410	64.78013265	82.55710532	298	415
PROPANE (g)	-104700	73.46589015	97.4880755	298	415
BENZENE (g)	82900	82.03002213	117.7739878	298	415
Heat Exchanger (FEHE)					
Species	**IN (kmol)**	**H (kJ)**	**OUT (kmol)**	**H (kJ)**	
PROPENE	84.65	1755289.57	84.65	2457324.19	
PROPANE	9.00	-952653.25	9.00	-852292.74	
BENZENE	185.46	9739427.08	185.46	17542389.62	
ΔH (GJ/h)	**8.60535767**				

Table A.7 Energy balance of the hot stream across the heat exchanger (FEHE)

Heat Exchanger (FEHE)					
IN (S-107)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPANE (l)	-119800	119.6	--	298.15	503
PROPANE (g)	-104700	73.46589015	113.2468631	298.15	503
BENZENE (l)	49000	135.69	--	298.15	503
BENZENE (g)	82900	82.03002213	139.6519746	298.15	503
CUMENE (l)	-41200	214.4	--	298.15	503
CUMENE (g)	4000	149.4010399	242.626238	298.15	503
OUT (S-108)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPANE (l)	-119800	119.6	--	298.15	308
BENZENE (l)	49000	135.69	--	298.15	308
CUMENE (l)	-41200	214.4	--	298.15	308
Species	**IN (kmol)**	**H (kJ)**	**OUT (kmol)**	**H(kJ)**	
PROPANE	9	-797994.1384	9	-1067597.46	
BENZENE	100.95	8678023.016	100.95	5081474.369	
CUMENE	84.38	705985.9696	84.38	-3298258.941	
ΔH (GJ)	**-7.870396879**				

Table A.8 Energy balance across Flash Tank (V-101)

Flash Tank V-101						
OUT (S-108)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**	
PROPANE (l)	-119800	119.6	--	298.15	308	
BENZENE (l)	49000	135.69	--	298.15	308	
CUMENE (l)	-41200	214.4	--	298.15	308	
OUT (S-109)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**	
PROPANE (g)	-104700	73.47	100.33	298.15	430	
BENZENE (g)	82900	82.03	121.81	298.15	430	
CUMENE (g)	4000	149.40	212.34	298.15	430	
OUT (S-110)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**	
PROPANE (l)	-119800	119.6	--	298.15	430	
BENZENE (l)	49000	135.69	--	298.15	430	
CUMENE (l)	-41200	214.4	--	298.15	430	
Species	**IN (kmol)**	**H (kJ)**	**OUT (S-109) [kmol]**	**H (kJ)**	**OUT (S-110) [kmol]**	**H (kJ)**
PROPANE	9.00	-1067597.46	8.90	-829857.01	0.10	-10403.07
BENZENE	100.95	5081474.37	90.48	8716698.13	10.47	700345.91
CUMENE	84.38	-3298258.94	53.00	1475930.16	31.38	-405786.08
ΔH (GJ)	**8.931**					

Table A.9 Energy balance across Heat Exchanger (E-101)

Heat Exchanger - 101

IN (S-109)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (g)	-104700.00	73.47	100.33	298.15	430
BENZENE (g)	82900.00	82.03	121.81	298.15	430
CUMENE (g)	4000.00	149.40	212.34	298.15	430
OUT (S-111)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPANE (l)	-119800.00	119.60	--	298.15	298.15
BENZENE (l)	49000.00	135.69	--	298.15	298.15
CUMENE (l)	-41200.00	214.40	--	298.15	298.15
Species	**IN (kmol)**	**H (kJ)**	**OUT (kmol)**	**H (kJ)**	
Benzene	8.90	-829857.01	8.90	-1066220	
Cumene	90.48	8716698.13	90.48	4433520	
Propane	53.00	1475930.16	53.00	-2183600	
ΔH (GJ)	**-8.179**				

Table A.10 Energy balance across Flash Tank (V-102)

Flash Tank V-102					
IN (S-111)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPANE (l)	-119800	119.60	--	298.15	298.15
BENZENE (l)	49000	135.69	--	298.15	298.15
CUMENE (l)	-41200	214.40	--	298.15	298.15
OUT (S-112)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**
PROPANE (g)	-104700	73.47	84.62	298.15	351
BENZENE (g)	82900	82.03	99.01	298.15	351
CUMENE (g)	4000	149.40	174.92	298.15	351

OUT (S-113)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.60	--	298.15	351
BENZENE (l)	49000	135.69	--	298.15	351
CUMENE (l)	-41200	214.40	--	298.15	351

Species	IN (kmol)	H (kJ)	OUT (S-112) [kmol]	H (kJ)	OUT (S-113) [kmol]	H (kJ)
PROPANE	8.90	-1066220	4.32	-434257.57	4.58	-519734.46
BENZENE	90.48	4433520	2.71	237623.88	87.77	4930147.67
CUMENE	53.00	-2183600	0.17	2114.30	52.83	-1578030.92
ΔH (GJ)	**1.454**					

Table A.11 Energy balance across Heat Exchanger (E-103)

Heat Exchanger - 103

IN (S-110)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.6	--	298.15	430
BENZENE (l)	49000	135.69	--	298.15	430
CUMENE (l)	-41200	214.4	--	298.15	430

OUT (S-114)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.6	--	298.15	354
BENZENE (l)	49000	135.69	--	298.15	354
CUMENE (l)	-41200	214.4	--	298.15	354

Species	IN (kmol)	H (kJ)	OUT (kmol)	H (kJ)
PROPANE	0.10	-10403.07	0.10	-11312.03
BENZENE	10.47	700345.91	10.47	592374.66
CUMENE	31.38	-405786.08	31.38	-917104.35
ΔH (GJ)	**-0.6202**			

Table A.12 Energy balance across benzene distillation column (T-101)

Distillation Column (T-101)							
IN (S-115)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**		
PROPANE (l)	-119800	119.60	--	298.15	352		
BENZENE (l)	49000	135.69	--	298.15	352		
CUMENE (l)	-41200	214.40	--	298.15	352		
OUT (S-116)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**		
PROPANE (l)	-119800	119.60	--	298.15	340		
BENZENE (l)	49000	135.69	--	298.15	340		
CUMENE (l)	-41200	214.40	--	298.15	340		
OUT (S-117)	**ΔH_f (kJ/kmol)**	**$C_{P,0}$ (kJ/kmol*K)**	**C_P (kJ/kmol*K)**	**T_0 (K)**	**T (K)**		
PROPANE (l)	-119800	119.60	--	298.15	456		
BENZENE (l)	49000	135.69	--	298.15	456		
CUMENE (l)	-41200	214.40	--	298.15	456		
Species	IN (S-115)	H (kJ)	OUT (S-116)	H (kJ)	OUT (S-117)	H (kJ)	
PROPANE	4.67	-529389.05	4.67	-536091.44	0.00	0.00	
BENZENE	98.23	5531027.43	98.22	5370534.69	0.01	704.19	
CUMENE	84.21	-2497210.50	0.00	0.00	84.21	-619529.60	
ΔH (GJ)	**1.711**						

Table A.13 Energy balance across cumene distillation column (T-102)

Distillation Column (T-102)

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IN (S-117)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.60	--	298.15	456
BENZENE (l)	49000	135.69	--	298.15	456
CUMENE (l)	-41200	214.40	--	298.15	456

OUT (S-118)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.60	--	298.15	456
BENZENE (l)	49000	135.69	--	298.15	456
CUMENE (l)	-41200	214.40	--	298.15	456

OUT (S-119)	ΔH_f (kJ/kmol)	$C_{P,0}$ (kJ/kmol*K)	C_P (kJ/kmol*K)	T_0 (K)	T (K)
PROPANE (l)	-119800	119.60	--	298.15	483
BENZENE (l)	49000	135.69	--	298.15	483
CUMENE (l)	-41200	214.40	--	298.15	483

Species	IN (S-117) [kmol]	H (kJ)	OUT (S-118) [kmol]	H (kJ)	OUT (S-119) [kmol]	H (kJ)
PROPANE	0.00	0.00	0.00	0.00	0.00	0.00
BENZENE	0.01	704.19	0.01	704.19	0.00	0.00
CUMENE	84.21	-619529.60	84.11	-618793.91	0.10	-156.82
ΔH (kJ)	**578.9**					

Data Retrieved from Perry’s Handbook and the NIST database [19,20].

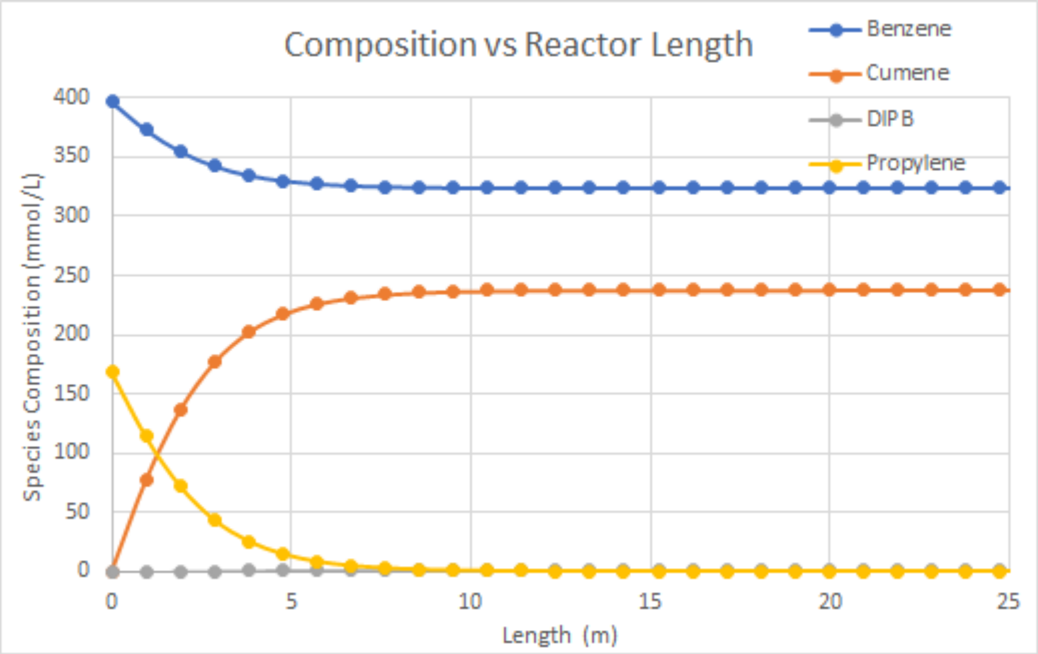

Figure A.2 Change in species composition across the length of the PFR in SuperPro.

Table A.14 Heat of Vaporization Values for All Process Components

Species	Enthalpy of Vaporization (kJ/kmol)
Benzene	30548.24
Cumene	36849.23
p-DIBP	50892
Propane	18945.29
Propene	18623.55

Table A.15 Temperature-Dependent Density Values for All Process Components

Species	Density (kg/m^3) [=a + bT] (T in K)

	a	b
Benzene	1171.66	-1.0017
Cumene	1108.25	-0.8356
p-DIBP	860	0
Propane	969.89	-1.606
Propene	1029.33	-1.7663

Equipment Sizing Heuristics

For calculating the area of the heat exchanger, either Equation A.5 or A.6 would be used for different conditions. If a phase change occurs, Equation A.5 would be used, where λ would be the enthalpy of vaporization of the stream.

$$Q = m\lambda \tag{A.5}$$

In the case that no phase change occurs, the following equation could be used to calculate the heat transfer:

$$Q = mC_p\Delta T \tag{A.6}$$

To determine the area of heat exchanger, the heat transfer calculated from one of the previous two equations can be equated to:

$$Q = U \cdot F \cdot A \cdot \Delta T_{1M} \tag{A.7}$$

For certain cases, there are specific values of the overall heat transfer coefficient. Specific values of U included 850 W/m^2 C for when a stream was condensed, and 1140 W/m^2 C for when the heat exchanger is a reboiler. ΔT_{lm} is the logarithmic mean temperature difference. The shape factor, F, can range from 0.8 to 0.9, but 0.9 was used for all of the heat exchanger calculations. For calculating the shaft power of a pump, it can be done by using:

$$W_s = 1.67 \cdot \frac{(volumetric\ flow\ rate) \cdot \Delta P}{e} \tag{A.8}$$

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The efficiency of the pump ranges from 0.6 to 0.7. An efficiency of 0.7 would be used for calculating the shaft power of every pump. Calculating the shaft power of a compressor requires a different equation:

$$W_s = \dot{m} \cdot z_1 \cdot R \cdot T_1 \cdot \frac{((P_2/P_1)^a - 1)}{a} \tag{A.9}$$

$$a = \frac{k-1}{k} \tag{A.10}$$

$$k = \frac{C_P}{C_V} \tag{A.11}$$

When sizing the compressors, it was assumed that the gaseous multi-component stream behaved as an ideal gas. This would mean that the compressibility factor, z_1, would be equal to 1 and that $C_p = C_v + R$. The efficiency would also need to be taken into account to figure out the actual amount of shaft power needed. The efficiency calculated from the equation below is for an electric powered compressor.

$$x_{dr}(\%) = 75 + 11.5 \log W_s - 1.5(\log W_s)^2 \tag{A.12}$$

$$x_{dr}(\%) = -18 + 36 \log W_s - 3(\log W_s)^2 \tag{A.13}$$

In the equation above, it would be used for finding the efficiency of a steam powered compressor. In the case that Equation A.9 results in more than 100 kW needed for the compressor, a steam powered compressor would be more favorable over an electric powered compressor. For the sizing of vessels, more specifically the flash tanks, Equation A.14 would be used, where the velocity of the gas would be calculated. In the flash tanks for this production process, the vapor-liquid stream would be separated into two streams: a vapor and a liquid stream. In this process, a k value of 0.0305 was used because it was assumed that the vessels did not have mesh entrainers.

$$u\,(m/s) = k\sqrt{\frac{\rho_l}{\rho_v} - 1} \tag{A.14}$$

The gas velocity can be used to calculate the diameter of the vessel. The volume of the liquid occupying half of the vessel and the volume occupied by a 5 minute liquid flow can be used to calculate the length of the vessel. However, the L/D ratio needs to be between 2.5 and 5. In the case that L/D is not within the range, the length can be found by multiplying a number between

2.5 to 5 with the diameter. For the reflux drum, finding the volume for a 5 minute liquid hold-up can be used to find the volume of the whole vessel, assuming that the tank would be half full during the hold-up. For calculating the number of trays in a distillation column, Fenske's equation and Antoine's equation would be needed. To find the actual number of trays needed, the theoretical number of trays would be divided by the tray efficiency and multiplied by 1.1. The 1.1 is a safety factor for the number of trays. In sizing the plug-flow reactor, Equations 2 and 3 would be needed alongside the following equation to determine the volume of the reactor.

$$V = F_{Ao}\int_0^X \frac{1}{-r_A}dX \tag{A.15}$$

The calculations for the equipment sizing and specifications are demonstrated below from Tables A.16 to A.23. The tables present the values of the variables that would be plugged into the heuristic equations and/or be further applied with the heuristic relations explained above. The tables also present the calculations for equipment specifications such as the fluid density of the streams. The values highlighted in yellow are the calculated values that are tabulated in Tables 6, 7, and 8.

Equipment Sizing

Table A.16 Equipment Sizing for Heat Exchangers

E-101	S-4	m (kmol/h)	mol frac	ΔH (kJ/kmol)	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	185.4575	0.664484056	20298.81842	2059123.785	850	0.9	28.80935194
	Cumene	0.0001	3.58295E-07	0.013202877				
	p-DIBP	0	0	0	Duty (MJ/h)		A (m^2)	
	Propane	8.9974	0.032237191	610.7429317	7412.252647		93.43025431	
	Propene	84.645	0.303278395	5648.12035				
	Total	279.1	1	26557.6949				

E-102	S-9	m (kmol/h)	mol frac	ΔH (kJ/kmol)	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	90.4806	0.593635	18134.50444	-1357781.91	-850	0.9	63.70542598
	Cumene	53.0002	0.347729499	12813.56429				
	p-DIBP	3.97E-02	2.60E-04	13.25574227	Duty (MJ/h)		A (m^2)	
	Propane	8.8974	0.058375033	1105.931936	4887.62388		27.86070874	
	Propene	0	0	0				
	Total	152.4179	1	32067.2564				
E-103	S-17	m (kmol/h)	mol frac	ΔH (kJ/kmol)	Q (W)	U (reboiler)	F	ΔT (lm)
	Benzene	0.0084	9.95829E-05	3.042083465	863990.7393	1140	0.9	97.00196128
	Cumene	84.2101	0.998320131	36787.32811				
	p-DIBP	0.1333	0.001580286	80.42393405	Duty (MJ/h)		A (m^2)	
	Propane	0	0	0	3110.117852		8.681228977	
	Propene	0	0	0				
	Total	84.3518	1	36870.79413				

E-104	S-19	m (kmol/h)	mol frac	Cp (kJ/kmol*C)	ΔT (C)	U (g to g)	F	ΔT (lm)
	Benzene	0	0	0	26.858	30	0.9	56.36655371
	Cumene	0.099	1	221.6186				
	p-DIBP	-	-	-	Duty (MJ/h)		Q (W)	A (m^2)
	Propane	0	0	0	1.382703577		384.1150537	0.252392288
	Propene	0	0	0				
	Total - p-DIBP	0.099	1	221.6186				
	Total + p-DIBP	0.2323						
E-105	S-18	m (kmol/h)	mol frac	ΔH (kJ/kmol)	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	0.0084	9.98579E-05	3.050484323	-861092.736	-850	0.9	56.79081581
	Cumene	84.1111	0.999900142	36845.55031				
	p-DIBP	0.00E+00	0.00E+00	0	Duty (MJ/h)		A (m^2)	
	Propane	0	0	0	3099.685875		19.82030727	
	Propene	0	0	0				

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	Total	84.1195	1	36848.6008				
E-106	S-10	m (kmol/h)	mol frac	ΔH	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	10.4652	0.2489521	7605.048915	-411870.1609	-850	0.9	79.5346
	Cumene	31.3782	0.7464424	27505.82841				
	p-DIBP	0.0936	0.0022266	113.3166306	Duty (MJ/h)		A (m^2)	
	Propane	0.1	0.0023789	45.06813046	1482.61397		6.76928486	
	Propene	0	0	0				
	Total	42.037	1	35269.26208				
E-107	S-16	m (kmol/h)	mol frac	ΔH	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	98.2234	0.9545752	29160.59182	-858153.6377	-850	0.9	57.82564
	Cumene	0.0001	9.718E-07	0.035811589				
	p-DIBP	0	0	0	Duty (MJ/h)		A (m^2)	
	Propane	4.674	0.0454238	860.5678997	3089.105967		19.39917157	
	Propene	0	0	0				
	Total	102.8975	1	30021.19553				

E-108	S-18	m (kmol/h)	mol frac	ΔH	Q (W)	U (cond)	F	ΔT (lm)
	Benzene	0.0084	9.986E-05	3.050484323	-861092.736	-850	0.9	157.2749
	Cumene	84.1111	0.9999001	36845.55031				
	p-DIBP	0	0	0	Duty (MJ/h)		A (m^2)	
	Propane	0	0	0	3099.685875		7.156966625	
	Propene	0	0	0				
	Total	84.1195	1	36848.6008				

Table A.17 Equipment Sizing for Pumps

P-101 A/B	S-1	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ ρ	Fluid ρ (kg/m^3)	Q (m^3/h)	Q (m^3/min)
	Benzene	0	0	298.15	873.003145	0	502.0852223	7.48551348	0.12475856
	Cumene	0	0	298.15	859.11586	0			
	p-DIBP	0	0	298.15	860	0	ΔP (bar)	Efficiency	Ws (kW)
	Propane	196.45	0.05227006	298.15	491.0611	0.000106443	1.087	0.7	0.3235328
	Propene	3561.9157	0.94772994	298.15	502.707655	0.001885251			

	Total	3758.3657	1			0.001991694			
P-102 A/B	S-2	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	Fluid ρ (kg/m^3)	Q (m^3/h)	Q (m^3/min)
	Benzene	7030.2276	1	298.15	873.003145	0.001145471	873.003145	8.052923567	0.13421539
	Cumene	0	0	298.15	859.11586	0			
	p-DIBP	0	0	298.15	860	0	ΔP (bar)	Efficiency	Ws (kW)
	Propane	0	0	298.15	491.0611	0	1.087	0.7	0.34805694
	Propene	0	0	298.15	502.707655	0			
	Total	7030.2276	1			0.001145471			
P-103 A/B	S-16	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	Fluid ρ (kg/m^3)	Q (m^3/h)	Q (m^3/min)
	Benzene	7672.5847	0.973838216	340.2633	830.8182524	0.001172144	810.4203507	9.721752043	0.1620292
	Cumene	0.012	1.52309E-06	340.2633	823.9259865	1.84858E-09			
	p-DIBP	0	0	340.2633	860	0	ΔP (bar)	Efficiency	Ws (kW)
	Propane	206.109	0.026160261	340.2633	423.4271402	6.17822E-05	0.5	0.7	0.19327769

	Propene	0	0	340.2633	428.3229332	0			
	Total	7878.7057	1			0.001233928			

Table A.18(a) Equipment Sizing for Compressors

C-101 A/B	S-6	m (kmol/h)	mol frac	Cp (J/mol*K)	Cv (J/mol*K)	k	a	m (mol/s)	z1	R (J/mol*K)	T1 (K)
	Benzene	100.9458	0.51947802	74.83793097	70.51899071	1.04605449	0.044026851	54.019599	1	8.314	523.15
	Cumene	84.3784	0.434220385	108.6051992	104.995091						
	p-DIBP	-	-	-	-	P2 (bar)	P1 (bar)	Ws (kW)		Efficiency	Ws (actual)
	Propane	8.9974	0.046301595	5.39617413	5.01122267	15	25	118.6822529		0.4376866	271.15807
	Propene	0	0	0	0						
	Total - p-DIBP	194.3216	1	188.8393043	180.5253043						
	Total + p-DIBP	194.455									
C-102 A/B	S-18	m (kmol/h)	mol frac	Cp (J/mol*K)	Cv (J/mol*K)	k	a	m (mol/s)	z1	R (J/mol*K)	T1 (K)
	Benzene	0.0084	9.98579E-05	0.012089788	0.011259569	1.04100371	0.039388626	23.3683971	1	8.314	469.69
	Cumene	84.1111	0.999900142	211.0640737	202.7509039						
	p-DIBP	-	-	-	-	P2 (bar)	P1 (bar)	Ws (kW)		Efficiency	Ws (actual)

	Propane	0	0	0	0	2.7	2.2	18.76381631		0.8721117	21.515381
	Propene	0	0	0	0						
	Total - p-DIBP	84.1195	1	211.0761635	202.7621635						
	Total + p-DIBP	84.1195									

Table A.18(b) Calculating Fluid Density of Streams through Compressors

S-6 **(C-101 A/B)**	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ
Benzene	7885.2461	0.427490204	523.15	647.620645	0.00066009
Cumene	10141.802	0.549826985	523.15	671.10586	0.00081929
p-DIBP	21.6394	0.001173157	523.15	860	1.3641E-06
Propane	396.7551	0.021509654	523.15	129.7111	0.00016583
Propene	0	0	523.15	105.290155	0
Total	18445.443	1			0.00164657
				Fluid ρ (kg/m^3)	607.323063
S-18 **(C-102 A/B)**	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ
Benzene	0.6589	6.51709E-05	469.69	701.171527	9.2946E-08

Cumene	10109.678	0.999934186	469.69	715.777036	0.00139699
p-DIBP	0.0065	6.42906E-07	469.69	860	7.4757E-10
Propane	0	0	469.69	215.56786	0
Propene	0	0	469.69	199.716553	0
Total	10110.344	1			0.00139708
				Fluid ρ (kg/m^3)	715.776141

Table A.19(a) Calculating Fluid Density of Vapor and Liquid Streams exiting Flash Tank V-101

V-101	S-9 (g)	m (kg/h)	mass frac	mass frac/MW	MW of vapor (g/mol)	P (atm)	R (J/mol*K)
	Benzene	7067.7702	0.510792161	0.00653906	90.78260111	2.6	8.314
	Cumene	6370.3189	0.460386921	0.003830365			
	p-DIBP	6.4462	0.000465871	2.87107E-06	T (K)		Fluid ρ of vapor (kg/m^3)
	Propane	392.3454	0.028355047	0.00064303	430.2792		65.98049924
	Propene	0	0	0			
	Total	13836.881	1	0.011015327			
	S-10 (l)	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	
	Benzene	817.4759	0.177382	430.2792	740.6493254	0.0002395	

	Cumene	3771.4833	0.8183644	430.2792	748.7087005	0.001093	
	p-DIBP	15.1932	0.0032967	430.2792	860	3.833E-06	
	Propane	4.4097	0	430.2792	278.8616048	0	
	Propene	0	0	430.2792	269.327849	0	
	Total	4608.5621	0.9990432			0.0013364	
					Fluid ρ of liq (kg/m^3)	748.2996	

Table A.19(b) Equipment Sizing for Flash Tank V-101

Vapor (find D)				
k	u (m/s)	u (actual)	m (kg/s)	D (m)
0.0305	0.098081208	0.07356091	3.843577972	1.004134
Liquid (find L)				
Coeff * L	5 min of liq flow	L (m)	L/D	L (m)
0.39595245	0.513226042	1.296181	1.290844939	5.020669
^ [=Vol of liq]			^ Not within range	

Table A.20(a) Calculating Fluid Density of Vapor and Liquid Streams exiting Flash Tank V-102

V-102	S-12 (g)	m (kg/h)	mass frac	mass frac/MW	MW of vapor (g/mol)	P (atm)	R (J/mol*K)

	Benzene	212.0025	0.501342613	0.006418089	58.68561526	1.6	8.314
	Cumene	20.2176	0.047810495	0.000397778			
	p-DIBP	0.0033	7.80383E-06	4.80934E-08	T (K)		Fluid ρ of vapor (kg/m^3)
	Propane	190.6461	0.450839089	0.010224036	351.2769		32.15081845
	Propene	0	0	0			
	Total	422.8695	1	0.017039951			
	S-13 (l)	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	
	Benzene	6855.7677	0.5110901	351.2769	819.7859293	0.0006234	
	Cumene	6350.1013	0.4733932	351.2769	814.7230224	0.000581	
	p-DIBP	6.4429	0	351.2769	860	0	
	Propane	201.6993	0.0150365	351.2769	405.7392986	3.706E-05	
	Propene	0	0	351.2769	408.8696115	0	
	Total	13414.011	0.9995197			0.0012416	
					Fluid ρ of liq (kg/m^3)	805.44434	

Table A.20(b) Equipment Sizing for Flash Tank V-102

Vapor (find D)				
k	u (m/s)	u (actual)	m (kg/s)	D (m)

0.0305	0.149580854	0.11218564	0.11746375	0.20363
Liquid (find L)				
Coeff * L	5 min of liq flow	L (m)	L/D	L (m)
0.01628338	1.387847937	85.2309489	418.5573632	1.018151
^ [=Vol of liq]			^ Not within range	

Table A.21 Equipment Sizing for Reflux Drums: V-103 and V-104

V-103	S-16	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	Fluid ρ (kg/m^3)			
	Benzene	7672.5847	0.973838216	340.2633	830.8182524	0.001172144	810.4203507			
	Cumene	0.012	1.52309E-06	340.2633	823.9259865	1.84858E-09				
	p-DIBP	0	0	340.2633	860	0	Hold-up of fluid	V (m^3)	D (m)	L (m)
	Propane	206.1099	0.026160261	340.2633	423.4271402	6.17822E-05	0.810146004	1.620292007	0.88266123	2.6479837
	Propene	0	0	340.2633	428.3229332	0	^ 5 min holdup time			
	Total	7878.7057	1			0.001233928				
V-104	S-18	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	Fluid ρ (kg/m^3)			
	Benzene	0.6589	6.51709E-05	456.2356	714.6487995	9.11929E-08	727.0187847			
	Cumene	10109.678	0.999934186	456.2356	727.0195326	0.001375388				

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	p-DIBP	0.0065	6.42906E-07	456.2356	860	7.47565E-10	Hold-up of fluid	V (m^3)	D (m)	L (m)
	Propane	0	0	456.2356	237.1756264	0	1.158881519	2.317763037	0.99453323	2.9835997
	Propene	0	0	456.2356	223.4810597	0	^ 5 min holdup time			
	Total	10110.344	1			0.00137548				

Table A.22(a) Equipment Sizing for Distillation Columns

T-101	P sat (Benzene)						α	Nmin	N (theoretical)
	A	B	C	T (K)	log (P sat)	Psat (mmHg)	7.221046801	1.690516072	3.381032144
	6.8603	1184.24	-55.578	398.28	3.40470301	2539.235663			
							Tray ε		N (actual)
	P sat (Cumene)						0.25		14.87654143
	A	B	C	T (K)	log (P sat)	Psat (mmHg)			
	7.0479	1529.2803	-58.5756	398.28	2.54610285	351.6437067	Stage Height (m)	Column Height (m)	
							0.4	5.950616573	
T-102	P sat (Benzene)						α	Nmin	N (theoretical)
	A	B	C	T (K)	log (P sat)	Psat (mmHg)	4.704698432	5.756425385	11.51285077

	6.8603	1184.24	-55.578	469.69	4.00059055	10013.60715			
							Tray ε		N (actual)
	P sat (Cumene)						0.625		20.26261735
	A	B	C	T (K)	log (P sat)	Psat (mmHg)			
	7.0479	1529.2803	-58.5756	469.69	3.32805876	2128.426996	Stage Height (m)	Column Height (m)	
							0.4	8.105046941	

Table A.22(b) Equipment Sizing for Distillation Columns

T-101	S-15	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	v (m^3/s)
	Benzene	7673.244	0.42575738	351.9482	819.1135	0.00051978	0.006204
	Cumene	10121.58	0.56160596	351.9482	814.1621	0.0006898	
	p-DIBP	21.6361	0.0012005	351.9482	860	1.3959E-06	D (m)
	Propane	206.109	0.01143616	351.9482	404.6612	2.8261E-05	0.140527
	Propene	0	0	351.9482	407.6839	0	
	Total	18022.57	1			0.00123923	
					Fluid ρ (kg/m^3)	806.951717	
T-102	S-17	m (kg/h)	mass frac	T (K)	Density (kg/m^3)	mass frac/ρ	v (m^3/s)

	Benzene	0.69	6.8022E-05	456.292	714.5923	9.519E-08	0.003875
	Cumene	10121.47	0.99779767	456.292	726.9724	0.00137254	
	p-DIBP	21.65	0.00213431	456.292	860	2.4818E-06	D (m)
	Propane	0	0	456.292	237.085	0	0.111056
	Propene	0	0	456.292	223.3814	0	
	Total	10143.81	1			0.00137512	
					Fluid ρ (kg/m^3)	727.211631	

Table A.23 Equipment Sizing for Plug-Flow Reactor

R-101	S-5	m (kmol/h)	mole frac	A	Ea (J/mol)	R (J/mol *K)	T (K)	k (mol/L *s)	rA (rxn rate)
	Benzene	185.4575	0.664484056	2.80E+07	104181	8.314	523.15	0.00110837	0.000223363
	Cumene	0.0001	0						
	p-DIBP	0	0	F (A0) [Benzene] (mol/s)	X	V (L)	V (m^3)	D (m)	L (m)
	Propane	8.9974	0.032237191	51.51597222	0.456	228331.43	228.33143	3.07485945	30.74859455
	Propene	84.645	0.303278395					[L/D = 10]	
	Total	279.1	0.999999642						

Table A.24 Raw Materials Market Prices and Total Costs

Raw Material	Price (USD/Mt)	Amount (Mt/year)	Cost ($/year)
Benzene (China)	1020.16	56242.08	57375866.48
Propylene (China)	1259.12	28494.88	35878566.64
Propane (China)	682.79	1571.6	1073071.94
Phosphoric acid (China)	806.37	960	774114.24
Average Market Prices from Mar-May 2021		Total ($M/y)	95.10

Raw Material Cost Sample Calculation

Benzene: $1020.16 /MT * 56,242.08 Mt/year = $57,375,866.48 / year

Table A.25 Non-discounted Profitability Criterion

End of Year (k)	Investment	dk	FCI - ∑dk	R	COMd	(R-COM-dk) x (1-t) + dk	Cash Flow	Cumulative Cash Flow
0	-0.82	--	8.18	--	--	--	-0.82	-0.82
1	-4.09	--	8.18	--	--	--	-4.09	-4.91
2	-5.73	--	8.18	--	--	--	-5.73	-10.64
3	--	1.23	6.96	132.31	121.38	7.53	7.53	-3.11
4	--	1.23	5.73	132.31	121.38	7.53	7.53	4.42
5	--	1.23	4.50	132.31	121.38	7.53	7.53	11.95
6	--	1.23	3.27	132.31	121.38	7.53	7.53	19.48
7	--	1.23	2.05	132.31	121.38	7.53	7.53	27.02
8	--	1.23	0.82	132.31	121.38	7.53	7.53	34.55
9	--	--	--	132.31	121.38	7.10	7.10	41.65
10	--	--	--	132.31	121.38	7.10	7.10	48.75
11	--	--	--	132.31	121.38	7.10	7.10	55.85
12	2.45	--	--	133.13	121.38	7.63	10.09	65.94

PBP = 1 + (-3.11 +2.45) / (-3.11 - 4.42) = **1.09 years**

CCR = ∑ Positive Cash Flows / ∑ Negative Cash Flows

= (7.53 + 7.53 +7.53 +... +7.10 + 10.09) / (0.82 + 4.09 + 5.73) = **7.20**

ROROI = Average Annual Net Profit / Fixed Capital Investment (FCI_L)

=(7.53 + 7.53 +7.53 +... +7.10 + 7.63) / 10 /8.182 - 1/10 *100 = **80.58%**

$COM_d = 0.180FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM})$

= 0.180 * 8,182,474 + 2.73 * 936,700 + 1.23 * (307,000 + 0 + 95,101,619.3) = **$121.38 M**

Fuel Credit = [(0.10 kmol cumene/hr * 5.00 GJ/kmol cumene) + (0.13 kmol p-DIBP/hr * 6.82 GJ/kmol p-DIBP)] *8,000 hrs/year * $3.16/GJ = **$35,053.25/year**

Straight-Line Depreciation (d_k^{SL}) = [FCI_L - S]/n

6 year d_k^{SL} = [8,182,474 - 0.1*8,182,474]/6 = **$1,227,366.55/year**

Table A.26 Discounted Profitability Criterion

End of Year	Non-discounted Cash Flow	Discounted Cash Flow	Discounted Cumulative Cash Flow
0	-0.82	-0.82	-0.82
1	-4.09	-3.72	-4.54
2	-5.73	-4.73	-9.27
3	7.53	5.66	-3.61
4	7.53	5.14	1.53
5	7.53	4.68	6.21
6	7.53	4.25	10.46
7	7.53	3.86	14.32
8	7.53	3.51	17.83
9	7.10	3.01	20.85
10	7.10	2.74	23.58
11	7.10	2.49	26.07
12	10.09	3.21	29.29

PVR = Present Value of All Positive Cash Flows / Present Value of All Negative Cash Flows

= (5.66 + 5.14 + 4.68 + … + 2.49 + 3.21) / (0.82 + 3.72 + 4.73) = **4.16**

DPBP = 1 + (-3.61 + 2.1707) / (-3.61 - 1.53 = **1.28 years**

The discounted cash flows were found by multiplying each cash flow by the discount factor (*P/F,i,n*), where *n* is the number of years after the start of the project.

Ex: At year 2, Discounted cash flow = -5.73 / 1.1^2 = **-4.73**

Error Analysis

Calculated C_A = 0.320 mol/L
Simulated C_A = 0.324 mol/L
Percent Error = | [(0.320 - 0.324) / (0.320)] | * 100% = 0.0125 * 100% = 1.25%

Table A.27 Bare Module Cost

Units	Bare Module Cost($)
C-101	1,600,000
C-102	698,800
E-101	239,000
E-102	93,000
E-103	194,000
E-104	194,000
E-105	35,000
E-106	100,000
E-107	92,300
E-108	100,000
P-101	29,900
P-102	29,900
P-103	29,900
R-101	1,160,000
T-101	96,800
T-102	171,000

V-101	1,900,000
V-102	127,000
V-103	20,300
V-104	23,400
Total	6,934,300

*All values calculated using Equipment Sizing Tables and CAPCOST and CEPCI 2019

Example Calculation for E-101 Bare Module Cost Using Turton et al. Appendix A

To find purchase cost of equipment C^o_p :

$$\log_{10} C_p^o = K_1 + K_2 \log_{10}(A) + K_3[\log_{10}(A)]^2 \tag{A.16}$$

Using Table A.1 from Turton et al. to find the floating head exchanger for K_1= 4.8306, K_2= -0.8509 and K_3 = 0.3187. A is the size parameter of the unit, for heat exchangers it is area:

$\log_{10}C^o_p = 4.8306 - 0.8509*\log_{10}(93.4) + 0.3187*[\log_{10}(93.4)]^2$

C^o_p = \$24,621

Use the following equation to find the pressure factor F_p :

$$\log_{10} F_P = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \tag{A.17}$$

And Table A.2 from Turton et al. to find values of C. Since pressure for this heat exchanger is P= 13 barg, use C values of C_1 = 0.03881, C_2 = -0.11272, C_3 = 0.08183:

$\log_{10}Fp = 0.03881 - 0.11272*\log_{10}13 + 0.08183*(\log_{10}13)^2$

Fp = 1.03463

Then use Turton et al. Table A.3 to find the material factor ID number for SS-shell/SS-tube which is 5. Then using Turton et al. Figure A.18 to find F_M = 2.75.

Use the following equation to find C_{BM}:

$$C_{BM} = C_p^o F_{BM} = C_p^o (B_1 + B_2 F_M F_P) \tag{A.18}$$

And use Table A.4 from Turton et al. to find $B_1 = 1.63$ and $B_2 = 1.66$:

$C_{BM} = 24{,}621 * (1.63 + 1.66*2.75*1.03463)$

C_{BM} (2001)= \$156,419

Then to consider inflation, use 2019 CEPCI = 607.5

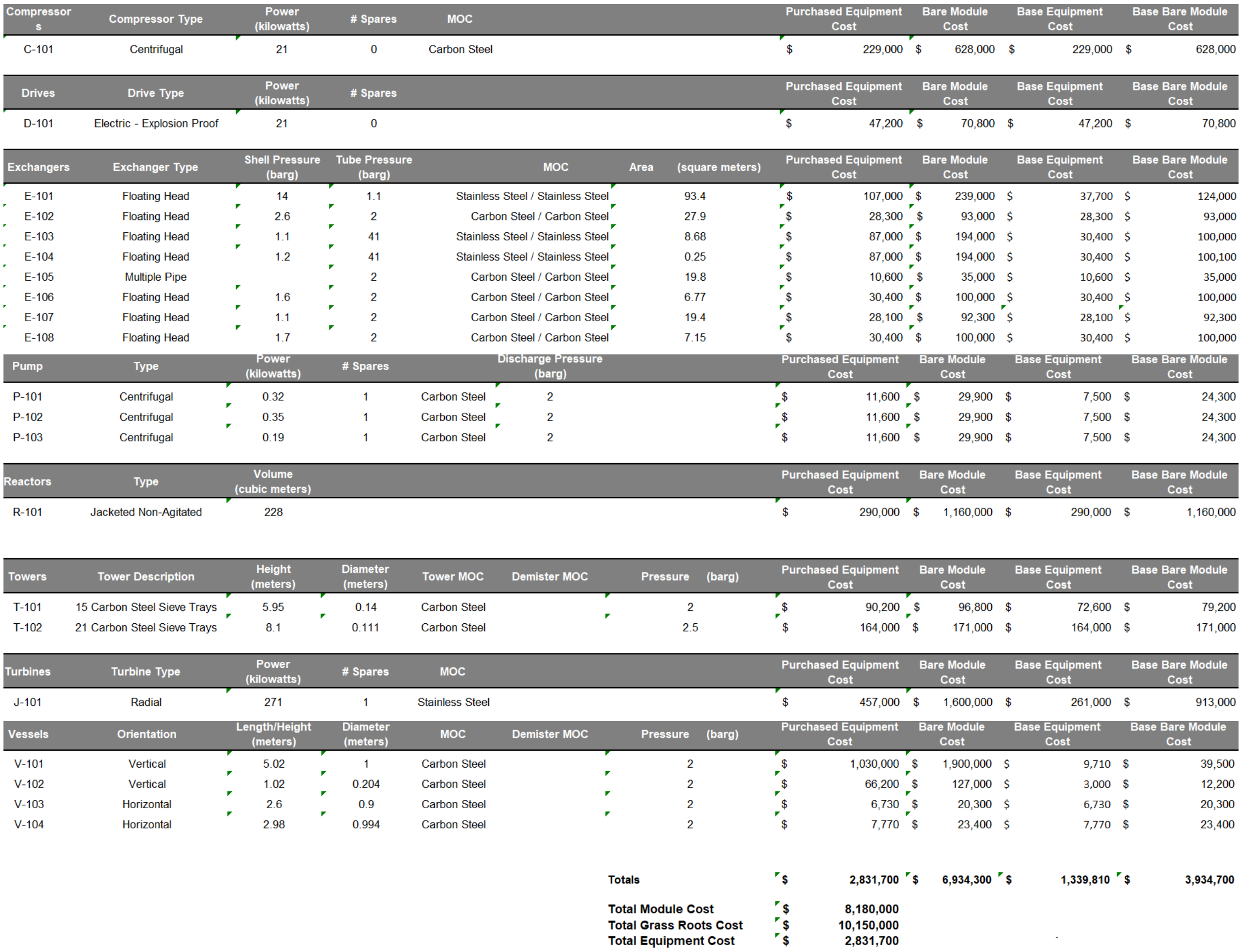
$C_{BM}(2019) = 156{,}419 *(607.5/397)$

C_{BM} = \$239,357

<u>Percent Error of Bare Module Cost compared to CAPCOST:</u>

% error = | [(239,000 - 239,357)/239,000] | x 100% = 0.15%

Table A.28 CAPCOST Values for Equipment in Cumene Process



Compressors	Compressor Type	Power (kilowatts)	# Spares	MOC	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
C-101	Centrifugal	21	0	Carbon Steel	$ 229,000	$ 628,000	$ 229,000	$ 628,000

Drives	Drive Type	Power (kilowatts)	# Spares	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
D-101	Electric - Explosion Proof	21	0	$ 47,200	$ 70,800	$ 47,200	$ 70,800

Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
E-101	Floating Head	14	1.1	Stainless Steel / Stainless Steel	93.4	$ 107,000	$ 239,000	$ 37,700	$ 124,000
E-102	Floating Head	2.6	2	Carbon Steel / Carbon Steel	27.9	$ 28,300	$ 93,000	$ 28,300	$ 93,000
E-103	Floating Head	1.1	41	Stainless Steel / Stainless Steel	8.68	$ 87,000	$ 194,000	$ 30,400	$ 100,000
E-104	Floating Head	1.2	41	Stainless Steel / Stainless Steel	0.25	$ 87,000	$ 194,000	$ 30,400	$ 100,100
E-105	Multiple Pipe		2	Carbon Steel / Carbon Steel	19.8	$ 10,600	$ 35,000	$ 10,600	$ 35,000
E-106	Floating Head	1.6	2	Carbon Steel / Carbon Steel	6.77	$ 30,400	$ 100,000	$ 30,400	$ 100,000
E-107	Floating Head	1.1	2	Carbon Steel / Carbon Steel	19.4	$ 28,100	$ 92,300	$ 28,100	$ 92,300
E-108	Floating Head	1.7	2	Carbon Steel / Carbon Steel	7.15	$ 30,400	$ 100,000	$ 30,400	$ 100,000

Pump	Type	Power (kilowatts)	# Spares		Discharge Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
P-101	Centrifugal	0.32	1	Carbon Steel	2	$ 11,600	$ 29,900	$ 7,500	$ 24,300
P-102	Centrifugal	0.35	1	Carbon Steel	2	$ 11,600	$ 29,900	$ 7,500	$ 24,300
P-103	Centrifugal	0.19	1	Carbon Steel	2	$ 11,600	$ 29,900	$ 7,500	$ 24,300

Reactors	Type	Volume (cubic meters)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
R-101	Jacketed Non-Agitated	228	$ 290,000	$ 1,160,000	$ 290,000	$ 1,160,000

Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
T-101	15 Carbon Steel Sieve Trays	5.95	0.14	Carbon Steel		2	$ 90,200	$ 96,800	$ 72,600	$ 79,200
T-102	21 Carbon Steel Sieve Trays	8.1	0.111	Carbon Steel		2.5	$ 164,000	$ 171,000	$ 164,000	$ 171,000

Turbines	Turbine Type	Power (kilowatts)	# Spares	MOC	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
J-101	Radial	271	1	Stainless Steel	$ 457,000	$ 1,600,000	$ 261,000	$ 913,000

Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
V-101	Vertical	5.02	1	Carbon Steel		2	$ 1,030,000	$ 1,900,000	$ 9,710	$ 39,500
V-102	Vertical	1.02	0.204	Carbon Steel		2	$ 66,200	$ 127,000	$ 3,000	$ 12,200
V-103	Horizontal	2.6	0.9	Carbon Steel		2	$ 6,730	$ 20,300	$ 6,730	$ 20,300
V-104	Horizontal	2.98	0.994	Carbon Steel		2	$ 7,770	$ 23,400	$ 7,770	$ 23,400

	Purchased Equipment Cost	Bare Module Cost	Base Equipment Cost	Base Bare Module Cost
Totals	**$ 2,831,700**	**$ 6,934,300**	**$ 1,339,810**	**$ 3,934,700**

Total Module Cost	**$ 8,180,000**
Total Grass Roots Cost	**$ 10,150,000**
Total Equipment Cost	**$ 2,831,700**

<u>Utilities Sample Calculation for E-102</u>

Cost of refrigerated water = \$4.76/GJ

Duty of E-102 = 4887 MJ/h * 1GJ/1000MJ = 4.887 GJ/h

Plant operation hours = 8000h/y

C_{UT} = 4.887 GJ/h * \$4.76/GJ * 8000h/y

C_{UT} = \$186,096 per year

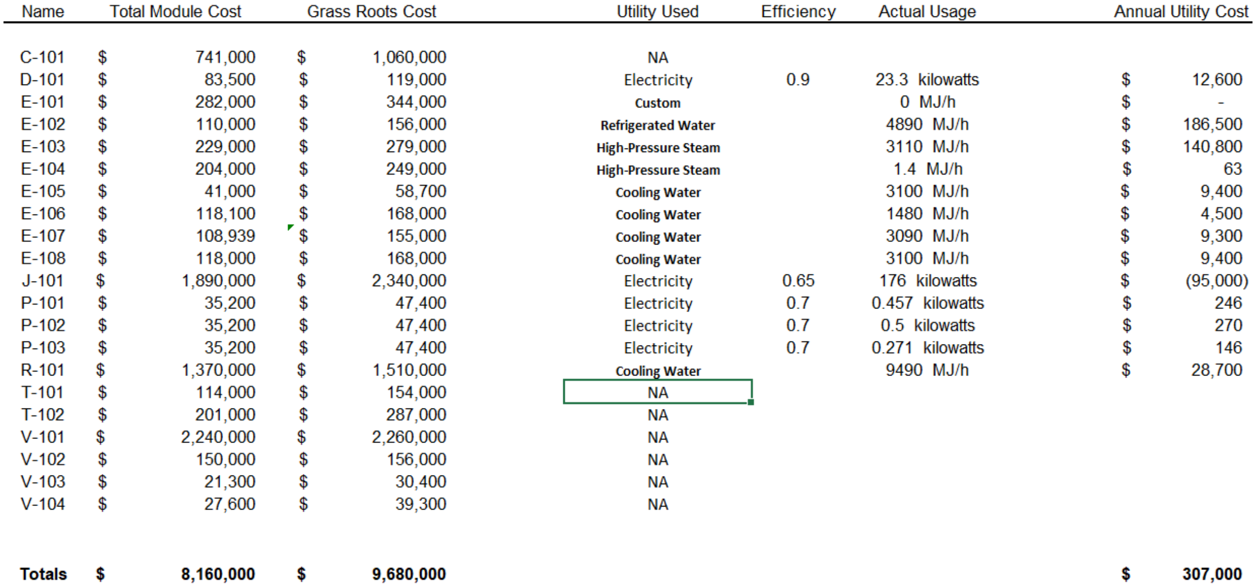
`

Percent Error of Cost of Utilities Compared to CAPCOST

% error = | [(186,096-185,500)/185,500] | x 100%

% error = 0.32%

Table A.29 CAPCOST Values for Cost of Utilities



Name	Total Module Cost	Grass Roots Cost	Utility Used	Efficiency	Actual Usage	Annual Utility Cost
C-101	$ 741,000	$ 1,060,000	NA			
D-101	$ 83,500	$ 119,000	Electricity	0.9	23.3 kilowatts	$ 12,600
E-101	$ 282,000	$ 344,000	Custom		0 MJ/h	$ -
E-102	$ 110,000	$ 156,000	Refrigerated Water		4890 MJ/h	$ 186,500
E-103	$ 229,000	$ 279,000	High-Pressure Steam		3110 MJ/h	$ 140,800
E-104	$ 204,000	$ 249,000	High-Pressure Steam		1.4 MJ/h	$ 63
E-105	$ 41,000	$ 58,700	Cooling Water		3100 MJ/h	$ 9,400
E-106	$ 118,100	$ 168,000	Cooling Water		1480 MJ/h	$ 4,500
E-107	$ 108,939	$ 155,000	Cooling Water		3090 MJ/h	$ 9,300
E-108	$ 118,000	$ 168,000	Cooling Water		3100 MJ/h	$ 9,400
J-101	$ 1,890,000	$ 2,340,000	Electricity	0.65	176 kilowatts	$ (95,000)
P-101	$ 35,200	$ 47,400	Electricity	0.7	0.457 kilowatts	$ 246
P-102	$ 35,200	$ 47,400	Electricity	0.7	0.5 kilowatts	$ 270
P-103	$ 35,200	$ 47,400	Electricity	0.7	0.271 kilowatts	$ 146
R-101	$ 1,370,000	$ 1,510,000	Cooling Water		9490 MJ/h	$ 28,700
T-101	$ 114,000	$ 154,000	NA			
T-102	$ 201,000	$ 287,000	NA			
V-101	$ 2,240,000	$ 2,260,000	NA			
V-102	$ 150,000	$ 156,000	NA			
V-103	$ 21,300	$ 30,400	NA			
V-104	$ 27,600	$ 39,300	NA			
Totals	**$ 8,160,000**	**$ 9,680,000**				**$ 307,000**

Table A.30 Major Equipment Specification for Optimized Process - SuperPro

Unit	Size	Amount	Total Cost ($)
Plug Flow Reactor (R-101)	289722 L	19	5,548,000
FEHE (E-101)	81.68 m^2	2	226,000
Flash Drum (V-101)	1873.87 L	8	80,000
Others			1,562,000
Total			7,416,000

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Table A.31 Major Equipment Specification for Alternative Process in Turton - SuperPro

Unit	Size	Amount	Total Cost ($)
Plug Flow Reactor	288383 L	25	7,300,000
FEHE	73.52 m^2	3	318,000
Flash Drum	1936.51 L	20	200,000
Others			2,044,000
Total			9,862,000

Table A.32 Rates of Consumption and Generation of Selected Reactants and Products - SuperPro

	Optimized Process (MT/yr)	Turton Process (MT/yr)
Benzene	55,679	139,708
Propylene	28,114	28,424
Cumene	80,001	80,000

Appendix B. Derivation of Equations

Reactor Conversion for Benzene

$a \cdot \text{Benzene} + b \cdot \text{Propylene} \rightarrow c \cdot \text{Cumene}$

a=1, b=1, c=1

$\mathbf{C_A = C_{A0} [(\theta_A + v_A x) / (1 + \varepsilon x)] (P / P_0) (T_0 / T)}$

$\theta_A = (F_{A0} / F_{A0}) = 1$

$\delta = [(c/a) - (b/a) - 1] = -1$

$y_{A0} = (F_{A0} / F_{T0}) = (55.2 \text{ mol/s} / 79.87 \text{ mol/s}) = 0.6911$

$\varepsilon = y_{A0}\,\delta = -0.6911$

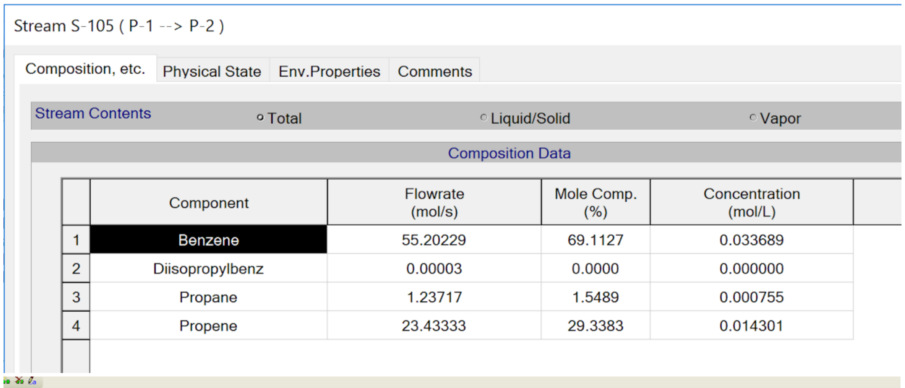
$\nu_A = -1$

$P_0 = 2.10$ bar, $P = 25.0$ bar

$T_0 = 245°C$, $T = 250°C$

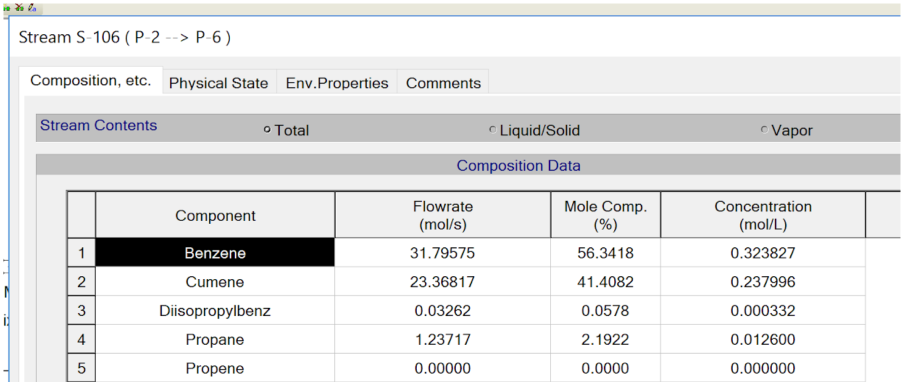
$x = 0.4239$ (benzene conversion)

$C_{A0} = 0.033689$ mol/L



Stream S-105 (P-1 --> P-2)

	Component	Flowrate (mol/s)	Mole Comp. (%)	Concentration (mol/L)
1	Benzene	55.20229	69.1127	0.033689
2	Diisopropylbenz	0.00003	0.0000	0.000000
3	Propane	1.23717	1.5489	0.000755
4	Propene	23.43333	29.3383	0.014301



Stream S-106 (P-2 --> P-6)

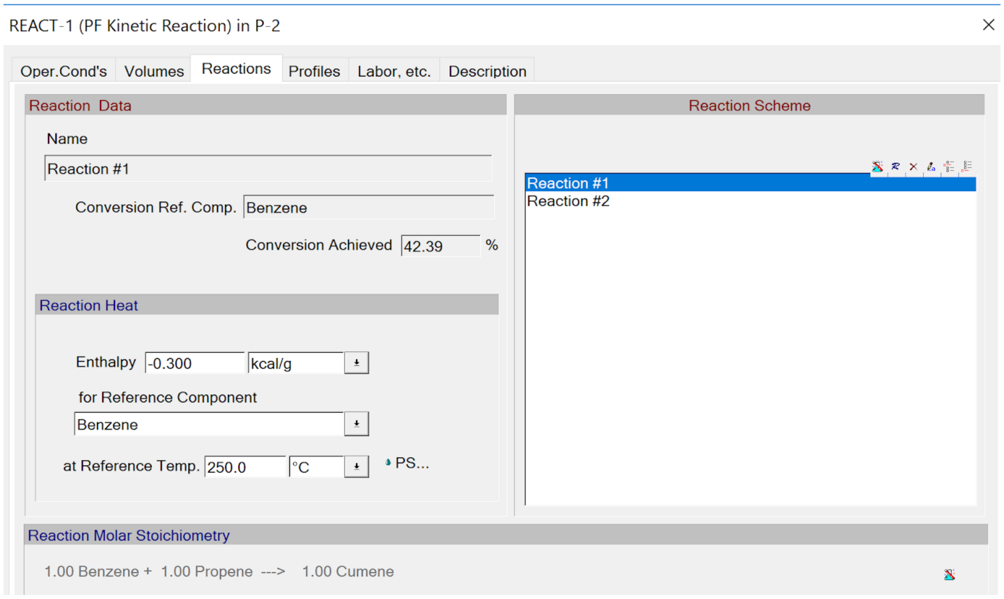
	Component	Flowrate (mol/s)	Mole Comp. (%)	Concentration (mol/L)
1	Benzene	31.79575	56.3418	0.323827
2	Cumene	23.36817	41.4082	0.237996
3	Diisopropylbenz	0.03262	0.0578	0.000332
4	Propane	1.23717	2.1922	0.012600
5	Propene	0.00000	0.0000	0.000000

$C_A = 0.033689 \text{mol/L} * [(1 + (-1*0.4239))/(1+(-0.6911*0.4239))] * (25 \text{ bar}/2.1 \text{ bar}) * (245°C/250°C)$

C_A = 0.320 mol/L (calculated)

C_A = 0.324 mol/L (simulated)

Conversion was calculated via SuperPro by inputting the kinetic data specific to the reaction with the catalyst in the PFR reactor, where X = 42.39%



REACT-1 (PF Kinetic Reaction) in P-2

Reaction Data

Name: Reaction #1

Conversion Ref. Comp.: Benzene

Conversion Achieved: 42.39 %

Reaction Heat

Enthalpy: -0.300 kcal/g

for Reference Component: Benzene

at Reference Temp.: 250.0 °C

Reaction #1
Reaction #2

Reaction Molar Stoichiometry

1.00 Benzene + 1.00 Propene ---> 1.00 Cumene

Appendix C. Tables of Data with Sources

Table C.1 Health and Fire Hazards data compiled from PubChem [7] [8] [17] [18] [19]

	Health Hazards	Fire Hazards
Propane	Vaporizing liquid may cause frostbite. High concentrations cause asphyxiation.	Extremely flammable.
Propylene	Moderate concentration in air causes dizziness, drowsiness and unconsciousness. Liquified propylene contact will cause 'freezing burn.'	Extremely flammable. Gas/air mixtures are explosive.
Benzene	Various health effects, ranging from dizziness and excitation to nausea and vomiting. Worse possible case involves coma and death. Carcinogenic, mutagenic.	Highly flammable. Vapor/air mixtures are explosive.
Cumene	Causes serious eye irritation, and may cause serious skin allergic reaction. Narcotic action with long-lasting effects, and depressant to the central nervous system.	Easily ignitable by sparks, heat or flames. Vapor/air mixtures are explosive.
p-DIPB	Causes skin irritation. Possibility of respiratory irritation, drowsiness/dizziness. Suspected of damaging fertility or unborn child.	

Table C.2 PEL, REL, TLV and IDLH data compiled from PubChem [7] [8] [17] [18] [19]

	Propane	Propylene	Benzene	Cumene	p-DIPB
Permissible Exposure Limits (PEL)	TWA: 1000 ppm		TWA: 1 ppm STEL: 5 ppm	TWA: 50 ppm	
Recommended Exposure Limit (REL)	1000 ppm (10hr avg.)		TWA: 0.1 ppm STEL: 1 ppm	TWA: 50 ppm	
Threshold Limit Values (TLV)	TWA: 1000 ppm	TWA: 500 ppm	TWA: 0.5 ppm STEL: 2.5 ppm	TWA: 50 ppm	
Immediately dangerous to life & health (IDLH)	2100 ppm		500 ppm	900 ppm	

Table C.3 LEL and UEL data compiled from PubChem. [7] [8] [17] [18] [19]

	Propane	Propylene	Benzene	Cumene	p-DIPB
Lower Explosive Limit (LEL)	2.1%	2%	1.2%	0.9%	
Upper Explosive Limit (UEL)	9.5%	11.1%	8%	6.5%	

Table C.4 Thermodynamic chemical properties to interpret environmental behavior. [10] [11] [12] [13] [14]

Chemical Species	Normal BP (°C)	MP (°C)	Henry's law constant (atm·m^3/mol)	K_{oc}	log(K_{ow})	BCF	Water solubility @ 25 °C (mg/ 100 mL)	Vapor Pressure @ 25 °C (kPa)
benzene	80.08	5.5	0.00556	85	2.13	1.1-20	1.8E-1	12.6
cumene	152.4	-96.0	0.01	~700	3.66	35.5	6.13E-4	0.60
diisopropylbenzene	~204	-57	~0.0204	~4000	unknown	~128-134	poor (no value found)	0.033-0.052
propylene/propene	-48	-185	0.196	~22	1.77	N/A	2.00E-3	1158

Table C.5 Heat capacity data from Perry's Handbook (8th Ed.) [20]

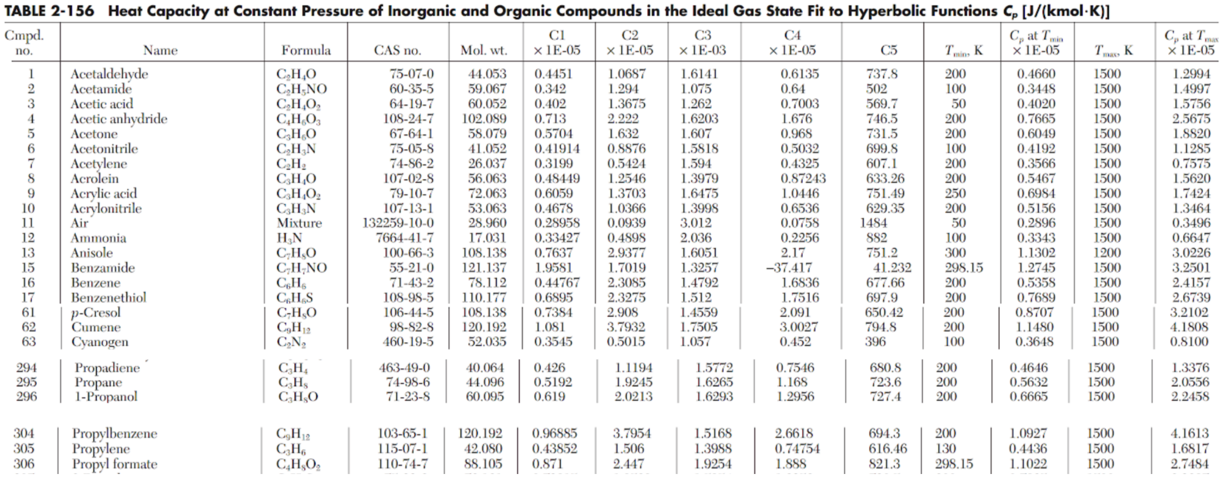


TABLE 2-156 Heat Capacity at Constant Pressure of Inorganic and Organic Compounds in the Ideal Gas State Fit to Hyperbolic Functions C_p [J/(kmol·K)]

Cmpd. no.	Name	Formula	CAS no.	Mol. wt.	C1 × 1E-05	C2 × 1E-05	C3 × 1E-03	C4 × 1E-05	C5	T_{min}, K	C_p at T_{min} × 1E-05	T_{max}, K	C_p at T_{max} × 1E-05
1	Acetaldehyde	C_2H_4O	75-07-0	44.053	0.4451	1.0687	1.6141	0.6135	737.8	200	0.4660	1500	1.2994
2	Acetamide	C_2H_5NO	60-35-5	59.067	0.342	1.294	1.075	0.64	502	100	0.3448	1500	1.4997
3	Acetic acid	$C_2H_4O_2$	64-19-7	60.052	0.402	1.3675	1.262	0.7003	569.7	50	0.4020	1500	1.5756
4	Acetic anhydride	$C_4H_6O_3$	108-24-7	102.089	0.713	2.222	1.6203	1.676	746.5	200	0.7665	1500	2.5675
5	Acetone	C_3H_6O	67-64-1	58.079	0.5704	1.632	1.607	0.968	731.5	200	0.6049	1500	1.8820
6	Acetonitrile	C_2H_3N	75-05-8	41.052	0.41914	0.8876	1.5818	0.5032	699.8	100	0.4192	1500	1.1285
7	Acetylene	C_2H_2	74-86-2	26.037	0.3199	0.5424	1.594	0.4325	607.1	200	0.3566	1500	0.7575
8	Acrolein	C_3H_4O	107-02-8	56.063	0.48449	1.2546	1.3979	0.87243	633.26	200	0.5467	1500	1.5620
9	Acrylic acid	$C_3H_4O_2$	79-10-7	72.063	0.6059	1.3703	1.6475	1.0446	751.49	250	0.6984	1500	1.7424
10	Acrylonitrile	C_3H_3N	107-13-1	53.063	0.4678	1.0366	1.3998	0.6536	629.35	200	0.5156	1500	1.3464
11	Air	Mixture	132259-10-0	28.960	0.28958	0.0939	3.012	0.0758	1484	50	0.2896	1500	0.3496
12	Ammonia	H_3N	7664-41-7	17.031	0.33427	0.4898	2.036	0.2256	882	100	0.3343	1500	0.6647
13	Anisole	C_7H_8O	100-66-3	108.138	0.7637	2.9377	1.6051	2.17	751.2	300	1.1302	1200	3.0226
15	Benzamide	C_7H_7NO	55-21-0	121.137	1.9581	1.7019	1.3257	−37.417	41.232	298.15	1.2745	1500	3.2501
16	Benzene	C_6H_6	71-43-2	78.112	0.44767	2.3085	1.4792	1.6836	677.66	200	0.5358	1500	2.4157
17	Benzenethiol	C_6H_6S	108-98-5	110.177	0.6895	2.3275	1.512	1.7516	697.9	200	0.7689	1500	2.6739
61	*p*-Cresol	C_7H_8O	106-44-5	108.138	0.7384	2.908	1.4559	2.091	650.42	200	0.8707	1500	3.2102
62	Cumene	C_9H_{12}	98-82-8	120.192	1.081	3.7932	1.7505	3.0027	794.8	200	1.1480	1500	4.1808
63	Cyanogen	C_2N_2	460-19-5	52.035	0.3545	0.5015	1.057	0.452	396	100	0.3648	1500	0.8100
294	Propadiene	C_3H_4	463-49-0	40.064	0.426	1.1194	1.5772	0.7546	680.8	200	0.4646	1500	1.3376
295	Propane	C_3H_8	74-98-6	44.096	0.5192	1.9245	1.6265	1.168	723.6	200	0.5632	1500	2.0556
296	1-Propanol	C_3H_8O	71-23-8	60.095	0.619	2.0213	1.6293	1.2956	727.4	200	0.6665	1500	2.2458
304	Propylbenzene	C_9H_{12}	103-65-1	120.192	0.96885	3.7954	1.5168	2.6618	694.3	200	1.0927	1500	4.1613
305	Propylene	C_3H_6	115-07-1	42.080	0.43852	1.506	1.3988	0.74754	616.46	130	0.4436	1500	1.6817
306	Propyl formate	$C_4H_8O_2$	110-74-7	88.105	0.871	2.447	1.9254	1.888	821.3	298.15	1.1022	1500	2.7484

Table C.6 Enthalpy data for species from Perry's Handbook. [20]

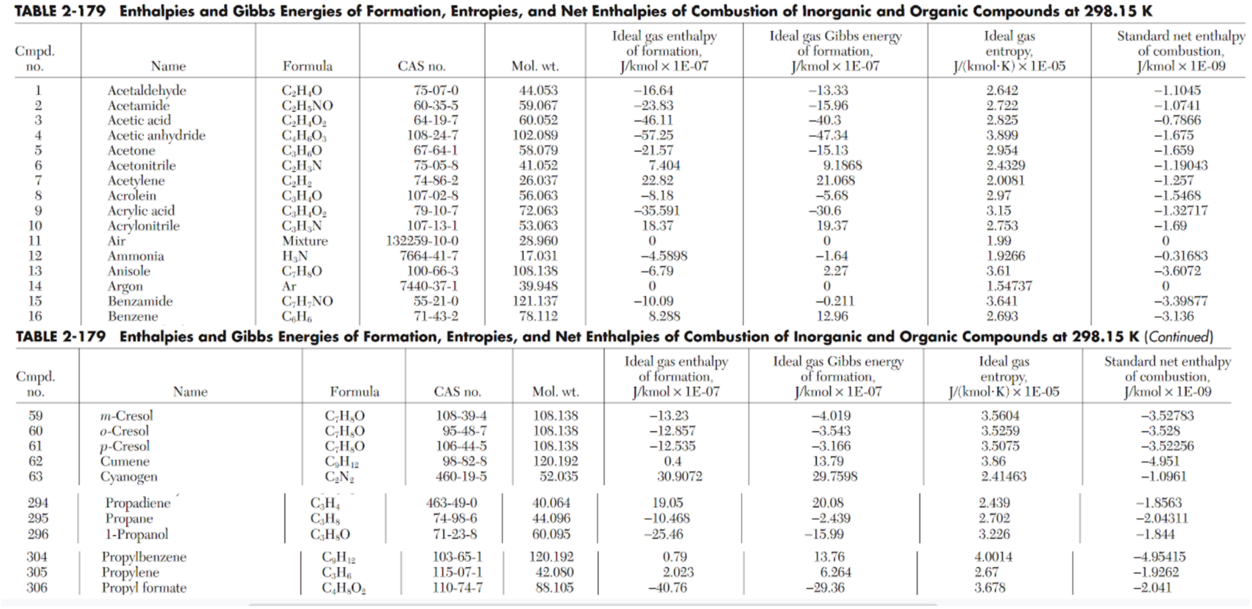


TABLE 2-179 Enthalpies and Gibbs Energies of Formation, Entropies, and Net Enthalpies of Combustion of Inorganic and Organic Compounds at 298.15 K

Cmpd. no.	Name	Formula	CAS no.	Mol. wt.	Ideal gas enthalpy of formation, J/kmol × 1E-07	Ideal gas Gibbs energy of formation, J/kmol × 1E-07	Ideal gas entropy, J/(kmol·K) × 1E-05	Standard net enthalpy of combustion, J/kmol × 1E-09
1	Acetaldehyde	C_2H_4O	75-07-0	44.053	−16.64	−13.33	2.642	−1.1045
2	Acetamide	C_2H_5NO	60-35-5	59.067	−23.83	−15.96	2.722	−1.0741
3	Acetic acid	$C_2H_4O_2$	64-19-7	60.052	−46.11	−40.3	2.825	−0.7866
4	Acetic anhydride	$C_4H_6O_3$	108-24-7	102.089	−57.25	−47.34	3.899	−1.675
5	Acetone	C_3H_6O	67-64-1	58.079	−21.57	−15.13	2.954	−1.659
6	Acetonitrile	C_2H_3N	75-05-8	41.052	7.404	9.1868	2.4329	−1.19043
7	Acetylene	C_2H_2	74-86-2	26.037	22.82	21.068	2.0081	−1.257
8	Acrolein	C_3H_4O	107-02-8	56.063	−8.18	−5.68	2.97	−1.5468
9	Acrylic acid	$C_3H_4O_2$	79-10-7	72.063	−35.591	−30.6	3.15	−1.32717
10	Acrylonitrile	C_3H_3N	107-13-1	53.063	18.37	19.37	2.753	−1.69
11	Air	Mixture	132259-10-0	28.960	0	0	1.99	0
12	Ammonia	H_3N	7664-41-7	17.031	−4.5898	−1.64	1.9266	−0.31683
13	Anisole	C_7H_8O	100-66-3	108.138	−6.79	2.27	3.61	−3.6072
14	Argon	Ar	7440-37-1	39.948	0	0	1.54737	0
15	Benzamide	C_7H_7NO	55-21-0	121.137	−10.09	−0.211	3.641	−3.39877
16	Benzene	C_6H_6	71-43-2	78.112	8.288	12.96	2.693	−3.136

TABLE 2-179 Enthalpies and Gibbs Energies of Formation, Entropies, and Net Enthalpies of Combustion of Inorganic and Organic Compounds at 298.15 K *(Continued)*

Cmpd. no.	Name	Formula	CAS no.	Mol. wt.	Ideal gas enthalpy of formation, J/kmol × 1E-07	Ideal gas Gibbs energy of formation, J/kmol × 1E-07	Ideal gas entropy, J/(kmol·K) × 1E-05	Standard net enthalpy of combustion, J/kmol × 1E-09
59	*m*-Cresol	C_7H_8O	108-39-4	108.138	−13.23	−4.019	3.5604	−3.52783
60	*o*-Cresol	C_7H_8O	95-48-7	108.138	−12.857	−3.543	3.5259	−3.528
61	*p*-Cresol	C_7H_8O	106-44-5	108.138	−12.535	−3.166	3.5075	−3.52256
62	Cumene	C_9H_{12}	98-82-8	120.192	0.4	13.79	3.86	−4.951
63	Cyanogen	C_2N_2	460-19-5	52.035	30.9072	29.7598	2.41463	−1.0961
294	Propadiene	C_3H_4	463-49-0	40.064	19.05	20.08	2.439	−1.8563
295	Propane	C_3H_8	74-98-6	44.096	−10.468	−2.439	2.702	−2.04311
296	1-Propanol	C_3H_8O	71-23-8	60.095	−25.46	−15.99	3.226	−1.844
304	Propylbenzene	C_9H_{12}	103-65-1	120.192	0.79	13.76	4.0014	−4.95415
305	Propylene	C_3H_6	115-07-1	42.080	2.023	6.264	2.67	−1.9262
306	Propyl formate	$C_4H_8O_2$	110-74-7	88.105	−40.76	−29.36	3.678	−2.041