

The University of Akron

IdeaExchange@UAkron

Williams Honors College, Honors Research
Projects

The Dr. Gary B. and Pamela S. Williams Honors
College

Spring 2023

Analysis of Plastic Pyrolysis Oil Separation using ChemCAD

Brian Berish
bdb100@uakron.edu

Juliana McGaffic
jgm78@uakron.edu

Follow this and additional works at: https://ideaexchange.uakron.edu/honors_research_projects

 Part of the [Petroleum Engineering Commons](#)

Please take a moment to share how this work helps you [through this survey](#). Your feedback will be important as we plan further development of our repository.

Recommended Citation

Berish, Brian and McGaffic, Juliana, "Analysis of Plastic Pyrolysis Oil Separation using ChemCAD" (2023). *Williams Honors College, Honors Research Projects*. 1678.
https://ideaexchange.uakron.edu/honors_research_projects/1678

This Dissertation/Thesis is brought to you for free and open access by The Dr. Gary B. and Pamela S. Williams Honors College at IdeaExchange@UAkron, the institutional repository of The University of Akron in Akron, Ohio, USA. It has been accepted for inclusion in Williams Honors College, Honors Research Projects by an authorized administrator of IdeaExchange@UAkron. For more information, please contact mjon@uakron.edu, uapress@uakron.edu.

Analysis of Plastic Pyrolysis Oil Separation using ChemCAD

CHEE:497-001 Honors Project



Prepared for

Dr. Newby, Dr. Gitiafroz, and Dr. Evans

By:

Juliana McGaffic and Brian Berish

April 21, 2023

Executive Summary

Problem Statement:

Pyrolysis technology and oil is an emerging market, there is an opportunity to capture value in recycling valuable products from waste plastic. A technical and economic analysis exploring the process of separating out valuable aromatic hydrocarbons from recycled plastic waste oil, known as pyrolysis oil, was conducted with the goal of understanding the separation technology and exploring potential profitable products. A ChemCAD simulation of the process was constructed to estimate the cost of the entire process.

Results:

Products derived from the pyrolysis oil feed are toluene/benzene fuel additive, recycled ethylbenzene monomer, recycled styrene monomer, and cumene. The process consists of three distillation towers, five cooling heat exchangers, one pump, and two steam ejector systems to create vacuum. A process flow diagram, equipment table, and stream table can be found in the results section of this report. Due to the monomer nature of the components, strict temperature limitations exist to prevent polymer formation in equipment. Therefore, vacuum distillation is used to keep monomer components under their polymerization point. Lack of accurate market value of the products at the distilled purity being investigated is the cause of reverse profitability and risk analyses, where the required revenue to achieve a certain likelihood of breaking even is used to estimate the overall project profitability. In addition, the safety concerns of distilling flammable, toxic, and carcinogenic components under vacuum brings a higher risk factor. Robust process safety design must be at the forefront of the full design of this process.

Implications:

The results from the project show it is impossible to sell recycled plastic monomers at a competitive price compared to virgin monomers in the current economic ecosystem. Therefore, it would be of great benefit to focus on recycling the most valuable components from the oil, while selling leftover material to refineries to be put into fuel. Extracting toluene and benzene from the pyrolysis oil would be a profitable fuel additive for high loaded engines and bio-diesel additive. This would be an efficient use of pyrolysis oil and provide an end-of-life use for plastic waste. This investigation strengthened distillation design principles involving vacuum distillation and materials at a high risk of polymerization. It strengthened our understanding of distillation tower design choices such as trays and reboiler orientation as it pertains to the project end goal. It also allowed us to further examine and understand the business considerations behind all industrial processes such as the profitability and risk analyses. Additionally, it allowed for additional safety considerations to be explored, such as the safety implications of excessive polymer fouling and runaway polymerization. These runaway polymerization events were further explored in a layers of protection analysis that helped strengthen our understanding of process safety.

Recommendations:

It is recommended to investigate the interest of refineries in buying pyrolysis oil products to solidify a market for this recycled fuel additive and recycled monomers for use in fuels. It is recommended to further investigate the safety implications of vacuum distillation using these components and apply it into an inherently safer plant design.

Introduction:

An overwhelming abundance of plastic waste has begun weighing on the collective global conscience. Since plastic's introduction into commercial and industrial use in the 1950's, the material has almost become ubiquitous in the developed and industrializing world. In 2015, it was estimated that the total amount of plastic produced since its invention was almost 5800 Megatons. 60% of this is currently in landfills across the globe where they will remain for hundreds of years (Geyer et al. 2017). Current popular forms of recycling include mechanical recycling, where plastic waste is ground down into a usable material, and incineration, where plastic waste is burned to produce energy. Mechanical recycling and incineration offer an alternative to landfills; however, chemical recycling offers an alternative that harnesses the natural energy dense nature of plastic waste and provides additional use. Pyrolysis is a form of chemical recycling where plastic waste is melted down into a petroleum-like oil where it can be separated into usable products (Qureshi et al. 2020).

The goal of this project is to explore the separation technology involved in the distillation of plastic pyrolysis oil. Usable products are derived from distilled product streams and the economics involved in the industrial implementation of the separation process are analyzed. The goal of this project was not to explore the chemical reaction involved in the creation of pyrolysis oil, but rather to confront the challenge of distillation in conditions that could cause spontaneous polymerization. As a result, recommendations with the goal to prevent polymer fouling, ensure personnel safety, and environmental safety are made.

Background:

Plastic is a material formed from a mixture of polymer molecules. A polymer is a long chain of repeating carbon-based molecules called monomers. These mixtures of long chain

molecules give plastic its unique qualities and allow it to readily resist natural degradation. The monomers are derived from crude oil and are reacted to form polymers in a process called polymerization. Plastic has proved to be a robust and economic material, allowing for solid and malleable applications while keeping manufacturing costs low. Over the course of the last fifty years, plastics and polymers have found their way into almost every facet of industrialized life. A combination of plastic's ubiquity and resistance to degradation has created a global excess of waste plastic (Reusch 2013).

Pyrolysis is the process of thermally degrading organic material or in the case of this study, plastic waste. The key factor in this process is the degradation that is performed in an oxygen free environment, preventing combustion of products. This preserves the chemical potential energy contained in the plastic waste and converts it down into base molecules. This is typically done in a reactor utilizing catalyst. The first step in this process is grinding the plastic waste up into fine particles and then sending the particles to the reactor to be heated to over 500 °C. Most plastic types degrade around the 450 to 500 °C range, therefore the reactor must operate at over 500 °C to account for different types of plastic. Three phases of products are created from pyrolysis. About 10% of the starting plastic waste is converted to solid char waste. This solid can be used as an asphalt additive or disposed of in a landfill. The liquid product is a hydrocarbon mixture that is the focus of this project. The vapor product is light hydrocarbon gases such as methane and butane, which can be recovered for fuel gas (Tullo 2022). The pyrolysis oil analyzed in this project is derived from polystyrene plastic waste (Polyflow 2009). Polystyrene is a hard and clear plastic found in hard plastic objects as well as packaging foam. It utilizes styrene as a monomer base, which is produced from ethylbenzene (Reusch 2013).

Pyrolysis is an emerging technology and faces several critical challenges. The first is the economic aspect of the process. Pyrolysis is an energy intensive process, which can rack up enormous utility costs. If the process is looking to make recycled plastic monomer feedstock, it is most likely impossible to compete with virgin feedstock due to the energy cost of operating a pyrolysis reactor and separation units. Plastic waste feedstock quality is also a major issue. Since the feed for the process is a mix of plastic waste, the correct types of plastic need to be sorted and pre-treated to be suitable for pyrolysis, adding additional energy and cost. Pre-treatment is also a major safety necessity to remove foreign objects and additives that have the potential to create toxic substances when undergoing high temperature degradation. Another issue is the stability of the product. Monomers can spontaneously polymerize under high temperature conditions. If monomers are present in the product mixture, then there is a risk of polymerization in storage, and it is necessary to invest in ways to prevent reaching those conditions. One final problem is the lack of analytical standards. Since the product is a mix of plastic molecules, there exists no metrics to easily measure and market pyrolysis product due to it coming from a mixture of plastic waste, instead of a well-established feedstock such as crude oil (Qureshi et al. 2020).

Despite the many challenges facing pyrolysis, it has several competitive advantages. The first is the ability to create a wide range of products. Once a reactor has been constructed, the catalyst and feed mixture can be swapped to change the product composition, allowing for flexibility in the market and the ability to meet market demand of specific products. A competitive advantage of pyrolysis is that it creates products that can be easily integrated into existing refinery infrastructure. Plastic and therefore pyrolysis oil are hydrocarbon based, therefore the molecules found in pyrolysis oil are found in the refinery technology chain,

meaning all that would be required is the ability to supply pyrolysis oil products into existing refinery infrastructure (Qureshi et al. 2020).

Methodology:

The first step is to conduct a simple topological optimization by sequencing separation units based on component relative volatility. The components in the feed mixture are identified and compiled into a feed stream using an existing pyrolysis oil composition. The data used is based on a Polyflow pyrolysis oil sample derived from polystyrene plastic waste (Polyflow 2009). The mole and weight percent of each component can be seen below in Table 1. The feed is high in toluene, ethylbenzene, and styrene; therefore, they will be the main products from separation. To give a quantitative value for the comparison of ease of separation, the relative volatilities of all components were compared. The largest relative volatilities between adjacent components indicate components that are most economical to separate. This is used as a guide to map out a series of separation units, and where specific components would be separated out. The relative volatilities of the components are shown below at 1 bar, the relative volatilities at 0.5 bar and 0.1 bar is in Appendix A table A.1, A.2, and A.3.

Table 1. Feed Stream Specifications

Component	Mole%	Weight%	BP at 1 atm (°C)	BP at 0.5 bar (°C)	BP at 0.1 bar (°C)		Relative Volatility at 1 bar
Benzene	6.15	4.77	80.1	58.8	20.0		
Toluene	27.69	25.35	110.6	87.6	45.3	Tol-Ben	1.60
Ethylbenzene	24.61	25.96	138.4	111.7	67.0	EB-Tol	2.05
Xylene	9.24	9.75	136	114.6	69.7	Xyl-EB	1.09
Styrene	27.69	28.65	145	120.5	75.1	Sty-Xyl	1.19
Cumene	4.62	5.52	152.4	127.0	80.9	Cum-Sty	1.22

(BP: boiling point)

Next, a ChemCAD model of the system is generated. To start, a shortcut distillation tower utilizing the Fenske-Underwood-Gilliland (FUG) method generates a design case for the minimum number of trays and the optimum feed location for a desired separation. The specifications to generate this case are the light key and heavy key split fractions. The light key split is the fraction of recovered material from the lighter (lower boiling point) component in the distillate. The heavy key split is the fraction of the heavier (higher boiling point) component recovered in the distillate. The light key and the heavy key are the components that make up the relative volatility. This process is repeated for each separation at 3 different pressures, atmospheric, 0.5 bar, and 0.1 bar using cold feed. Some components in feed are monomers and have the potential to polymerize inside the equipment with increased temperature. This must be avoided at all costs, therefore, to keep temperatures low, the towers are operated under reduced pressure.

Styrene has the potential to polymerize through thermal radical initiation. Since the polymerization reaction rate is proportional to the concentration of styrene monomer in the system, the separation temperature should decrease as the concentration of styrene increases due to other components being removed from the system (Zhao et al. 2019). In a 55/45 styrene/ethylbenzene system, the thermal initiation temperature is approximately 125 °C and in a system containing 100% styrene, the thermal initiation temperature is approximately 100 °C. For a system of 1 bar consisting of the initial feedstock, a temperature of 140 °C is suitable to prevent polymerization. As concentration of styrene increases, the tower pressure should decrease to achieve separation while decreasing the temperature.

The rigorous simultaneous correction distillation columns or SCDS columns were then generated for each separation at atmospheric, 0.5 bar, and 0.1 bar. The specifications for each

column or tower are set for 99% recovery of each light key and heavy key in the tops and bottoms, respectively. The method for pulling vacuum utilized in this design is a steam injector system. In a vacuum system, air leaks in all flanges across the vacuum process and the excess air is pulled through a pressure differential in the overhead off gas to create a vacuum effect (Turton et al, 2018). The sizing equations utilized for this injection nozzle are laid out in Appendix B.

To choose the most optimal design, equivalent annual operational cost (EAOC) is used to compare distillation designs. Data on distillation column condenser and reboiler duties must be collected at different tray and feed location settings to determine the most optimal case.

ChemCAD uses a sensitivity analysis where a certain independent variable can be varied in a specified range while recording dependent variables. For use in distillation tower optimization, the number of trays is the independent variable, and the tower reboiler and condenser duties are the dependent variables. These collected values on reboiler and condenser duties contribute to the EAOC calculation. Additionally, ChemCAD's sizing tool allows for the diameter of each tower case to be recorded based on tray specifications.

In addition to duties, the condenser and reboilers must be physically sized as well. The sizing is calculated using the overall heat transfer equation. An established overall heat transfer coefficients and log mean temperature difference are used with the calculated duty to solve for required heat transfer area. This gives an estimate for the exchanger size that works well for comparison cases and is laid out in Appendix B. Additionally, several product cooling exchangers and one feed cooler exchanger must be sized. This is done using ChemCAD's CCTherm tool, where the size of the exchanger is calculated based on the desired cooling utility, cooling tower water.

The EAOC optimization method estimates the best topological configuration for the tower systems by comparing both the purchase cost of the tower, trays, reboiler, and condensers as well as the annual utility costs. Using Equation 1 (Turton et al, 2018).

$$C_p^o = 10^{K_1 + K_2 * \log A + K_3 * (\log A)^2}$$

the purchase cost (C_p^o) can be estimated using correlations between purchase costs of equipment and a specific equipment size parameter. The data used to predict C_p^o was collected in 2003 then normalized to 2001, and in calculations, C_p^o was converted to 2022-dollar equivalent using chemical engineering plant cost index (CEPCI) conversion factors. All calculated values discussed are in a 2022-dollar equivalent unless indicated otherwise.

Table 2. Size parameters and corresponding units used to estimate the purchase cost of equipment investigated in project scope.

	Size Parameter	Units
Tower	Volume, V	m ³
Trays	Area, A	m ²
Heat Exchanger	Area, A	m ²
Pump	Shaft Power, W _s	kW

Table 3. CEPCI values used to convert all cost estimates to 2022-dollar equivalent.

Year	Index
2001	397
2022	836.2

The purchase cost of equipment is the first step in the module costing technique (Turton et al, 2018). The C_p^o calculated is for the base model of equipment constructed from carbon steel and operating under ambient temperatures. The bare module equipment cost (C_{BM}) is calculated from the C_p^o of the equipment and a bare module cost factor (F_{BM}), which accounts

for factors that may affect the purchase cost of equipment such as pressure factor, material of construction, contingency fees, and other indirect project expenses.

To compare the cost of building a new facility to adding this system to an existing plant, the grassroots cost (C_{GR}) and total module cost (C_{TM}). Equation 9 (Turton et al, 2018) is used to estimate C_{TM} assuming that the total module cost will be 18% higher than C_{BM} accounting for contingency costs and fees.

$$C_{BM} = C_p^o (B_1 + B_2 F_M F_P)$$

Equation 10 is used to estimate C_{GR} by assuming that the additional auxiliary facilities costs are equal to half the C_{BM} , and the C_{GR} is the total module cost plus the auxiliary facilities costs.

$$C_{GR} = C_{TM} + 0.5C_{BM}$$

The EAOC calculation for topological optimization also accounts for annual utility costs required to achieve product targets. Using utility estimates for low pressure steam and cooling water from Table 8.3 (Cum et al, 2018) and the required duties for condensers, reboilers, and supplementary heat exchangers, the annual utility costs for operation were calculated in terms of dollars per GJ of energy.

Table 4. Cost per GJ of energy provided by each utility used in ChemCAD model.

Utility	Value (\$/GJ)
Low Pressure Steam	2.78
Cooling Water	0.378

The capital cost annuity is calculated from C_{GR} to divide the cost of the equipment over its useful life and accounting for interest. The process is assumed to have a useful life of 20 years and an interest rate of 5%. Using Equation 11, the EAOC is calculated by summing the

capital cost annuity and the annual utility costs. The goal is to minimize the EAOC to find the least costly operation configuration.

$$EAOC = -(product\ value - feed\ cost - utility\ costs - waste\ treatment\ costs - capital\ cost\ annuity)$$

After determining the best operating configuration for the towers, the overall EAOC and profitability for the process can be calculated. Similar to the EAOC values used to optimize the towers, the overall EAOC accounts for purchase costs and the annual operating costs, however, the overall value includes the cost of labor, raw material costs, revenues, and the additional equipment need to reach product targets. The overall EAOC is calculated assuming an interest rate of 5% and a lifetime of 20 years.

Using the final topological optimization of the process, the annual labor cost can be calculated based on the number of unit operations present in the model. Equation 13 relates the number of particulate and nonparticulate processing units to the number of operators required per shift.

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5}$$

Assuming the process runs 24 hours and 7 days a week, 4.5 operators are hired for every operator required per shift giving the total number of operators to be hired. If the total number of operators hired is a decimal, the value is rounded up to the nearest whole number to provide excess operating support rather than too little. The total cost of labor is calculated using a salary of \$66,910 [2001] per operator and multiplied by the total number of operators for the process. This value contributes to the annual operating costs in the overall EAOC calculation.

The raw material costs are also accounted for in the annual operating costs of the overall EAOC calculation. The only raw material cost in the process is the purchase price of pyrolysis

oil which can be assumed to be very low, if not, negligible. The product selling prices account for the process revenues. Due to a lack of reliable sources of pricing for the products being sold, the risk analysis aims to determine the minimum selling price of the products to achieve a 50% likelihood of being profitable. The product prices will be determined as a function of the pure monomer price, using a scale factor to adjust the prices with the profitability of the process.

The risk analysis is performed first to calculate the product selling prices. A Monte-Carlo simulation was performed to quantify the risk associated with plant construction and operation. This simulation technique uses process parameters to generate a distribution of probabilities, identifying the likelihood of a range of net present values (NPV) of the process. Using the known parameters, an estimate for revenue is placed in the calculation assuming straight line depreciation and no salvage value. The revenue is then adjusted until there is a 50% likelihood of achieving a positive NPV. To calculate the sale price of the products, Excel Solver is used to adjust a scale factor for the products to reach the desired revenue. With the final revenues calculated, the overall EAOC is calculated to predict the profitability of the project.

Data and Results:

Separation sequencing yields three distillation columns. The first column, with toluene as the light key and ethylene benzene as the heavy key due to the largest relative volatility between pairs of close boiling points, pulls a mixture of benzene and toluene off the top of the tower. This accounts for 99% of the toluene in the feed and almost all the benzene due to it being lighter than toluene. The bottoms of the first tower flow to the second tower, which utilizes ethyl benzene as the light key and xylene as the heavy key and pulls 99% of the ethyl benzene present in its feed off the top of the tower, as well as half of the xylene present in the feed. This is due to xylene's boiling point being situated in between ethylbenzene and styrene. Xylene is only present in very

small amounts; therefore, it is not a viable product to pull from the feed. The remaining material in the bottoms flows to the third and final column where styrene is the light key and cumene as the heavy key, pulls 99% of the styrene to the top as well as the remaining xylene. The bottom collects the majority of the cumene in the feed. Figure 1 below visually represents the sequence of the separation units. Table A.1 in Appendix A shows the relative volatility data used to arrive at this result.

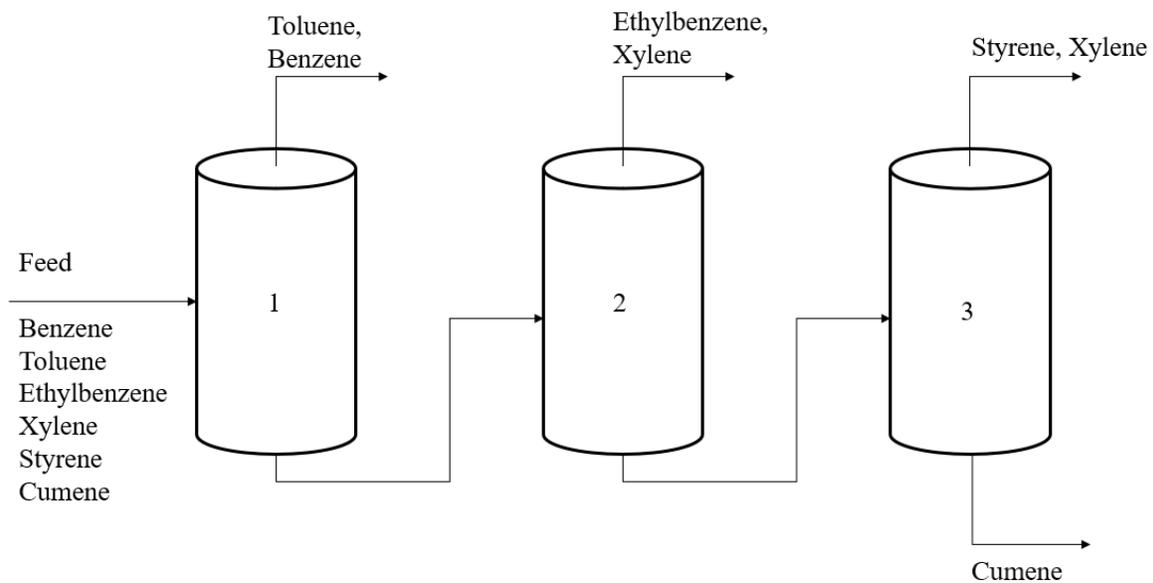


Figure 1: The results of the experimental sequencing of separation units based on the feed component’s relative volatilities.

The final process design is displayed in the process flow diagram in Figure 2 below. Tables 5 and 6 provide details of each major piece of equipment’s relevant specifications. Table 7 provides information on each stream in the process flow diagram.

P-101	T-101	E-101	T-102	E-102	E-103	T-103	E-104	E-105
Feed Pump	Toluene Separator	Toluene Cooler	Ethylbenzene Separator	Ethylbenzene Cooler	Separator Feed Cooler	Styrene Separator	Styrene Cooler	Cumene Cooler

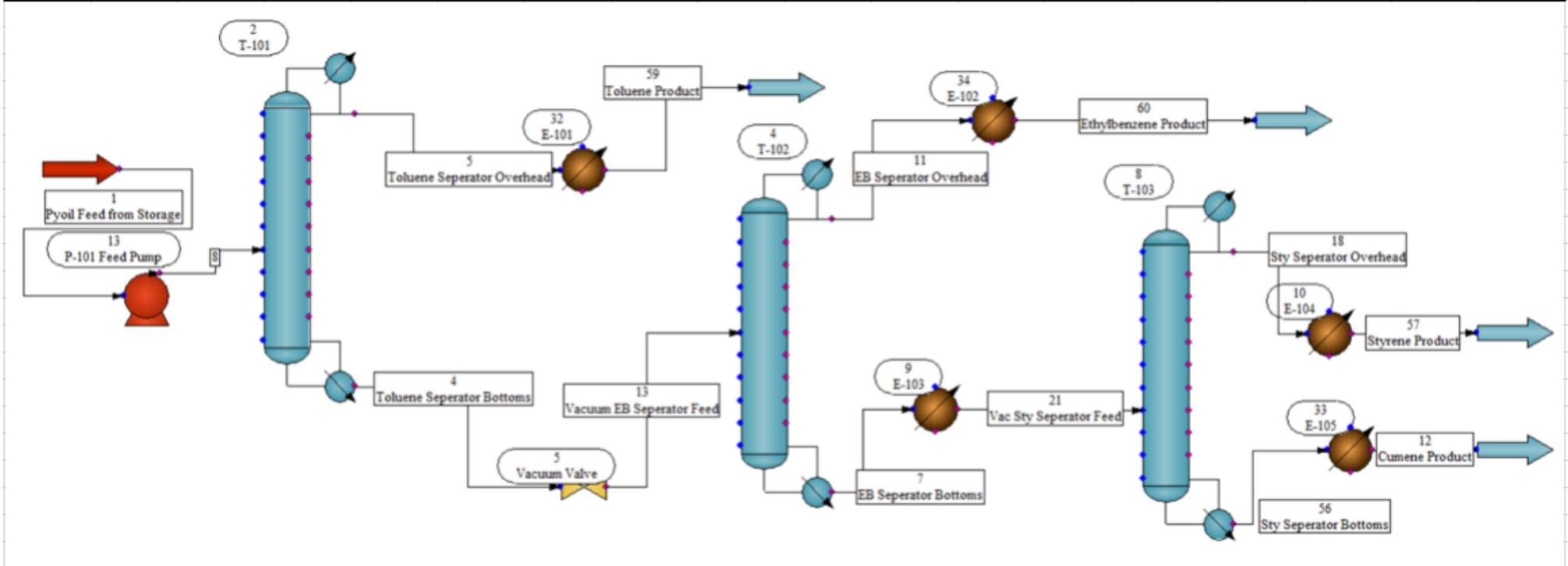


Figure 2: Process Flow Diagram for the Proposed Process

Table 5: Heat exchanger and pump equipment specifications

Heat Exchangers	
<p>E-101 Name: Toluene Product Cooler Area: 9.86 m² Type: Floating Head, Shell and Tube Material: Carbon Steel Process: Shellside Heat Utilized: 124.09 MJ/h Utility: Cooling Water</p>	<p>E-102 Area: 7.86 m² Type: Floating Head, Shell and Tube Material: Carbon Steel Process: Shellside Heat Utilized: 161.16 MJ/h Utility: Cooling Water</p>
<p>E-103 Name: Styrene Separator Feed Cooler Area: 2.06 m² Type: Floating Head, Shell and Tube Material: Carbon Steel Process: Shellside Heat Utilized: 106.56 MJ/h Utility: Cooling Water</p>	<p>E-104 Name: Styrene Product Cooler Area: 9.95 m² Type: Floating Head, Shell and Tube Material: Carbon Steel Process: Shellside Heat Utilized: 141.34 MJ/h Utility: Cooling Water</p>
<p>E-105 Name: Recycle Product Cooler Area: 6.39 m² Type: Floating Head, Shell and Tube Material: Carbon Steel Process: Shellside Heat Utilized: 53.4 MJ/h Utility: Cooling Water</p>	<p>Pumps</p> <p>P-101 Name: Feed Pump Type: Centrifugal/Electric Drive Material: Carbon Steel Power: 0.0192 kW Efficiency: 50% Pressure Out: 1 bar</p>

Table 6: Distillation tower specification table

Distillation Columns	
<p>T-101 Name: Toluene Separation Vessel: Carbon Steel 22 Carbon Steel Trays Feed Location: Tray 12 Tray Spacing: 0.61 m Column Height: 13.42 m Column Diameter: 0.91 m Reflux Ratio: 2.7 Weir Height: 0.05 m Operating Pressure: 1 bar</p>	<p>T-103 Name: Styrene Separator Vessel: Carbon Steel 62 Carbon Steel Trays Feed Location: Tray 34 Tray Spacing: 0.61 m Column Height: 37.21 m Column Diameter: 1.68 m Reflux Ratio: 10.4 Weir Height: 0.05 m Operating Pressure: 0.1 bar</p>
<p>T-102 Name: Ethylbenzene Separator Vessel: Carbon Steel 41 Carbon Steel Trays Feed Location: Tray 18 Tray Spacing: 0.61 m Column Height: 25.01 m Column Diameter: 1.83 m Reflux Ratio: 9.9 Weir Height: 0.05 m Operating Pressure: 0.1 bar</p>	

Table 7: Process Stream Table

Stream No.	1	8	5	59	4	13	7	11	60	21	18	57	56	12
Name	Pyoil Feed from Storage	Pyoil Feed	Toluene Separator Overhead	Toluene Product	Toluene Separator Bottoms	EB Separator Feed	EB Separator Bottoms	EB Separator Overhead	Ethyl Benzene Product	Vac Sty Separator Feed	Sty Separator Overhead	Styrene Product	Sty Separator Bottoms	Cumene Product
-- Overall --														
Temp C	25.0	25.0	102.8	35.0	141.0	72.0	75.4	67.2	35.0	60.0	74.8	35.0	80.4	35.0
Pres bar	0.9	1.1	1.0	1.0	1.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Vapor mole fraction	0	0	0	0	0	0.4	0	0	0	0	0	0	0	0
Molar flow kmol/h	30.0	30.0	10.2	10.2	19.8	19.8	11.3	8.6	8.6	11.3	9.8	9.8	1.5	1.5
Mass flow kg/h	3019.4	3019.4	910.6	910.6	2108.8	2108.8	1200.8	908.0	908.0	1200.8	1027.2	1027.2	173.5	173.5
Flow rates in kg/h														
Benzene	144.1	144.1	144.1	144.1	0	0	0	0	0	0	0	0	0	0
Ethylbenzene	784.0	784.0	7.8	7.8	776.1	776.1	7.8	768.4	768.4	7.8	7.8	7.8	0	0
M-Xylene	294.3	294.3	0.7	0.7	293.5	293.5	170.2	123.4	123.4	170.2	170.1	170.1	0.1	0.1
Cumene	166.6	166.6	0	0	166.6	166.6	166.5	0.0	0.0	166.5	1.7	1.7	164.9	164.9
Styrene	865.1	865.1	0.2	0.2	864.9	864.9	856.3	8.6	8.6	856.3	847.7	847.7	8.6	8.6
Toluene	765.4	765.4	757.7	757.7	7.7	7.7	0	7.7	7.7	0	0	0	0	0

Each tower is evaluated at three feed locations and across a range of total number of trays. The feed tray locations chosen to investigate more thoroughly were selected from the tower temperature profiles during the sensitivity analysis. The best three feed tray locations showed a smooth temperature profile and would provide similar technical performance. With similarities in technical performance, the EAO C was calculated at each feed tray location to evaluate which option would result in the lowest cost. Tower 1 (T-101) was evaluated at feed tray locations 10, 12, and 14 at atmospheric pressure across a range of 15 to 30 total trays. For each feed tray location, the EAO C generally decreased as the number of trays increased (Figure 3) due to reduced utility loads and condenser and reboiler sizing. The configuration resulting in the lowest EAO C for tower 1 is a total of 24 trays at feed tray 12. The column temperature profile is free of abnormalities and is viewable in Figure A.1 in Appendix A.

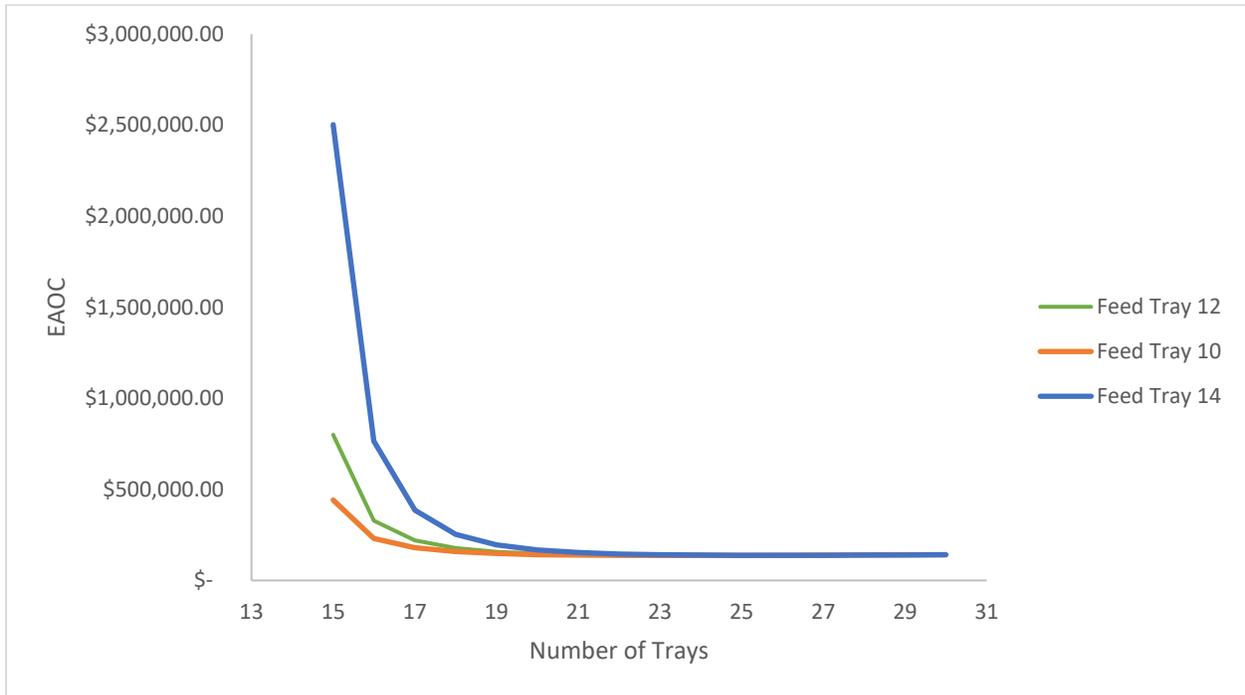


Figure 3. Comparison of EAO C trends as the total number of trays of T-101 increases for feed trays 10, 12, and 14.

For T-102, a similar comparison was performed, but multiple feed tray locations were evaluated at operating pressures of 0.5 bar and 0.1 bar. Multiple pressures were considered to account for the effects of increasing utilities from steam ejectors and comparing them against condenser and reboiler loads. Figure 4 below shows the relationship between the EAOC and the number of trays at each feed location for 0.5 bar. Figure 5 shows the relationship between EAOC and number of trays for each feed tray location at 0.1 bar. The optimal configuration for T-102 is 43 total trays at a feed location of tray 18 and an operating pressure of 0.1 bar. The temperature profile of the column is free of abnormalities and is viewable in Figure A.2 in Appendix A.

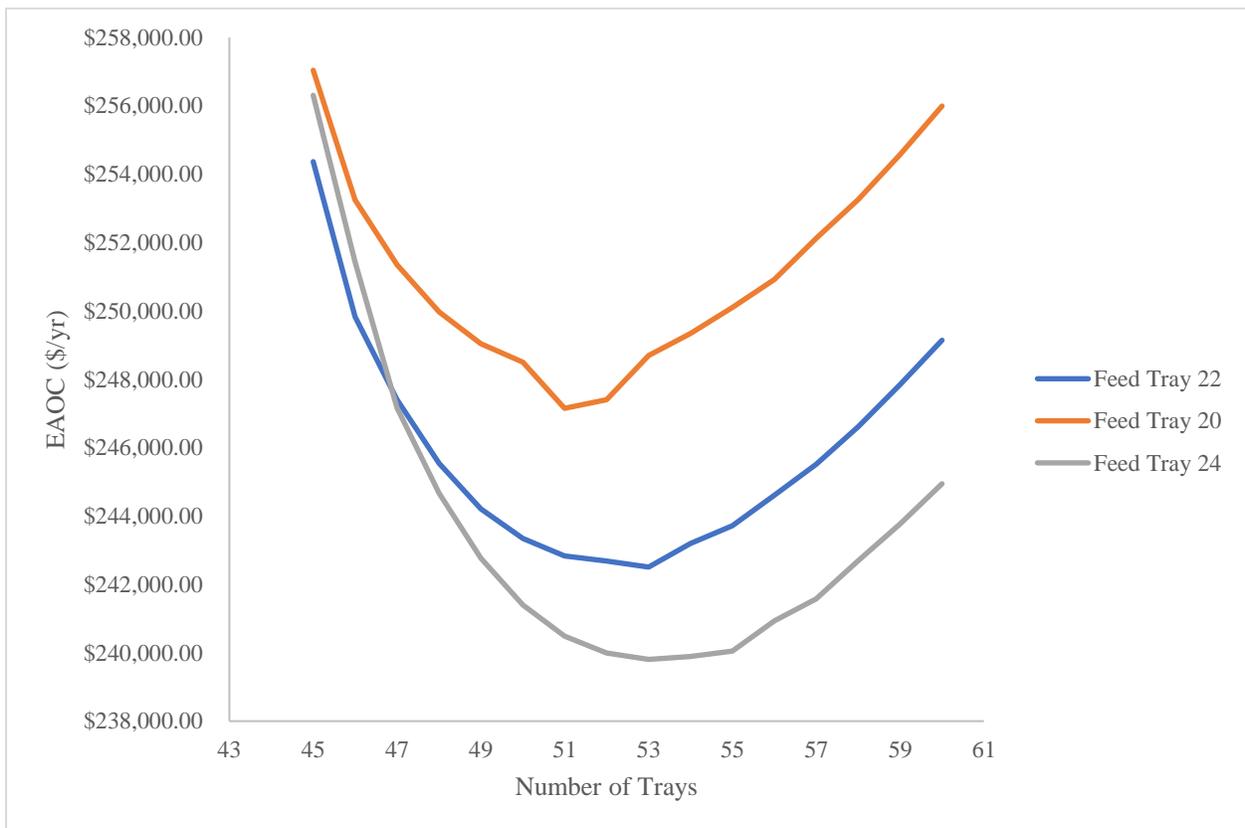


Figure 4. Comparison of EAOC trends as the total number of trays of T-102 increases for feed trays 22, 20, and 24 at an operating pressure of 0.5 bar.

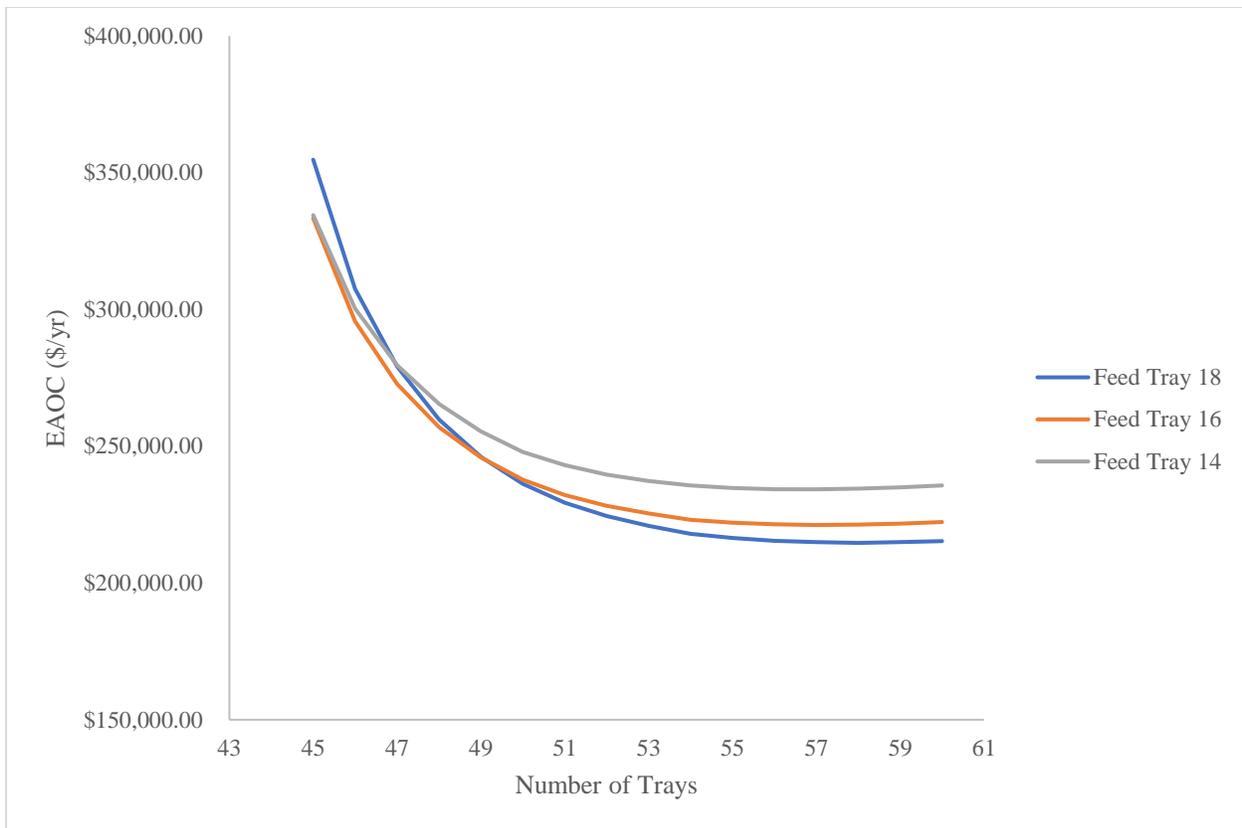


Figure 5. Comparison of EAO C trends as the total number of trays of T-102 increases for feed trays 18, 16, and 14 at an operating pressure of 0.1 bar.

Due to temperature constraints on styrene in T-103, the separation is limited to an operating pressure of 0.1 bar, where the temperature within the tower ranges from 75 to 80 °C, to avoid thermally initiating the polymerization of styrene and fouling trays. T-103 was evaluated at feed tray locations of tray 32, 30, and 34. The trend in EAO C seen in Figure 6 is inconsistent, which could likely be due to ChemCAD accounting for the pressure constraint. The optimal case for T-103 was decided to be 64 trays at a feed location at tray 34. A summary of the results of these EAO C comparisons can be found in Table 8.

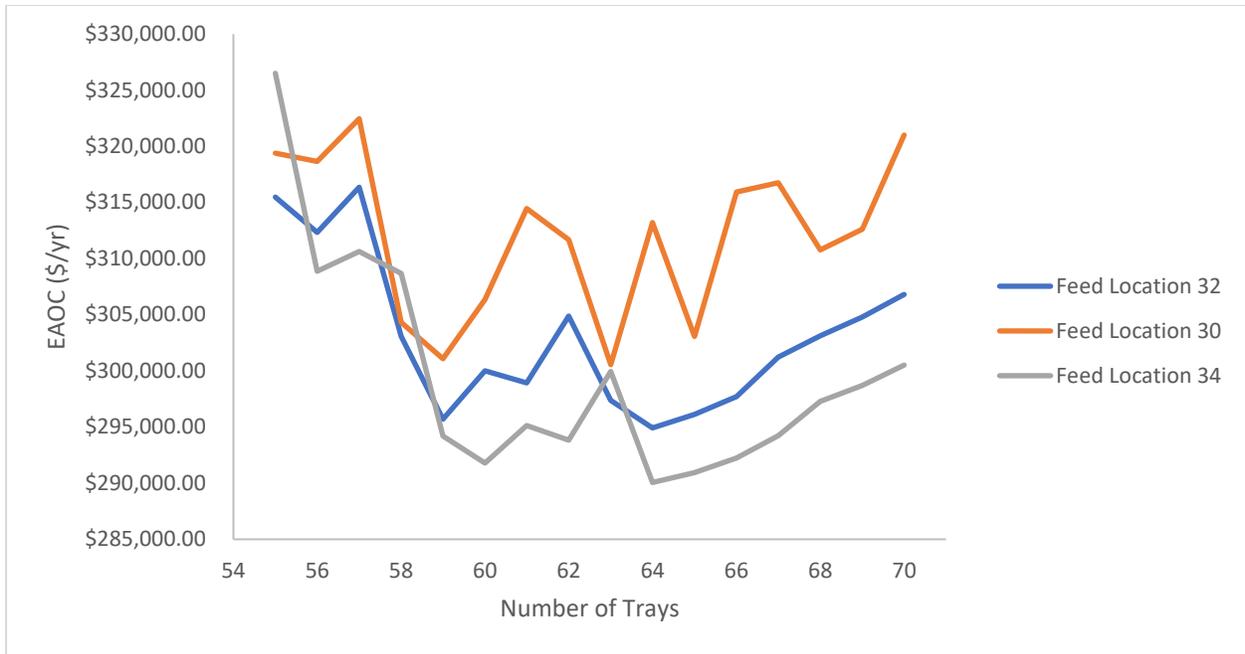


Figure 6. Comparison of EAOE trends as the total number of trays of T-103 increases for feed trays 32, 30, and 34 at an operating pressure of 0.1 bar.

Table 8. Summary of the optimized tower configuration producing the lowest EAOE.

	Pressure (bar)	Trays	Feed Tray
Tower 1 (T-101)	1	24	12
Tower 2 (T-102)	0.1	43	18
Tower 3 (T-103)	0.1	64	34

With the final tower configuration, additional equipment is added to achieve the best process conditions. Product coolers and pumps were added to the process and the corresponding equipment costs and utility costs were calculated for the overall EAOE and summarized in Tables 9 and 10.

Table 9. Summary of the sizing and costs associated with each product cooler.

	Duty (MJ/h)	Size (m ²)	CW Cost (\$/year)	Cap Cost Annuity (\$/yr)
Tower 1 Product Cooler	114.139	9.86	377.95	28,672
Tower 2 Product Cooler	53.130	7.93	175.93	30,261
Tower 3 Feed Cooler	47.114	2.91	156.01	45,941
Tower 3 Product Cooler	75.838	9.95	251.12	28,616
Tower 3 Recycle Cooler	42.734	7.98	141.50	30,208

Table 10. Summary of the sizing and costs with each pump added to the process.

	Shaft Power (MJ/hr)	Cap Cost Annuity (\$/yr)
Recycle Pump	1.95	3,980
Feed Pump	0.069	5,203

The overall EAOC uses all plant revenues and expenditures to evaluate the profitability of the process. The expenditures include purchase costs of equipment, utility costs, labor, and pyrolysis oil feedstock. The price of the pure monomers is scaled using a Monte-Carlo simulation, back calculating the selling price of the products to achieve a 50% likelihood of being profitable.

Calculations for labor costs revealed that a total of 13 operators are required to run the plant safely and efficiently, resulting in a labor cost of \$1,341,978 per year. The utility costs from all reboilers, condensers, and product coolers were summed to get the total yearly utility costs.

Table 11. Summary of expenditures contributing to EAOC calculation.

Expenditure	Cost (\$/yr)
Pyrolysis Oil	12,041,329
Total Cap Cost Annuity	537,072
Total Utility Cost	258,174
Labor	1,341,978

To determine the total revenue to achieve 50% likelihood of profitability, these expenditures are divided into the categories indicated in Table 12 to be used in the Monte-Carlo simulation. The revenue value acts as the independent variable in this calculation. For the minimum and maximum values of the Monte-Carlo simulation parameters, they were assumed to be 10% less than and 10% higher than the most likely value, respectively.

Table 12. Input parameters for Monte-Carlo simulation with dollar values shown in millions.

Parameter	Min (M\$)	Most Likely (M\$)	Max (M\$)
FCI,L	2.10	2.33	2.56
Revenues	12.60	14.00	15.40
Interest	4.5%	5%	5.5%
COMd	12.28	13.64	15.00
Taxes		0.5	
Salvage		0	

The most likely revenue value was adjusted until the final Monte-Carlo distribution showed a 50% likelihood of being profitable. The target revenue for this process is \$14 million. The results of the Monte-Carlo simulation can be seen in Figure 7. The pure monomer price is then scaled to be sold for a total \$14 million per year. The pure monomer price is multiplied by a scale factor of 0.387 to adjust the product prices. These prices can be seen in Tables 13 and 14

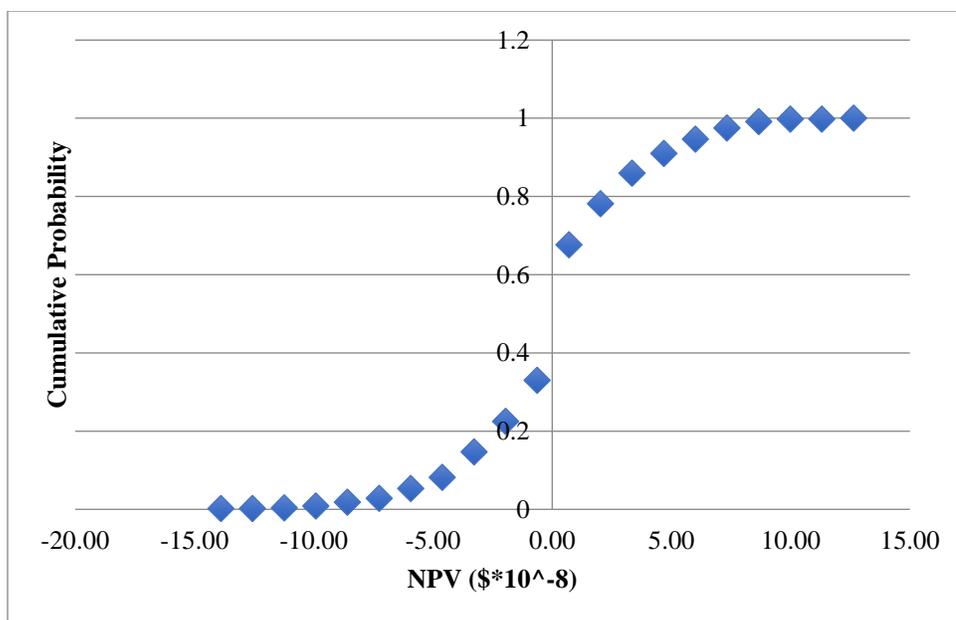


Figure 7. Final Monte-Carlo distribution with straight line depreciation after adjusting revenue to hit 50% likelihood of profitability target.

Table 13. Prices of pure monomers in dollars/kg.

Pure Monomer	Price (\$/kg)
Styrene	1.28
Ethylbenzene	1.83
Toluene	1.43
Cumene	1.34

Table 14. Prices of products after being scaled to revenue.

Product	Scaled Price (\$/kg)
Styrene	0.49
Ethylbenzene	0.71
Toluene	0.55
Cumene	0.52

The overall EAOC was calculated using the scaled product prices in Table 14, resulting in an optimized EAOC of \$178,553. This EAOC value indicates that this process is not profitable at the scaled product prices.

Discussion and Analysis:

The first product separated from the process is the majority toluene and benzene mix off the top of T-101. A strong market for this product would be as a high-octane gasoline or diesel additive. Octane is a rating that is an experimental standardized rating on the performance of a specific fuel. Octane rating is determined experimentally; therefore, it cannot be calculated theoretically. Octane is calculated using two methods, research octane number and motor octane number, which both measure engine knocking. Overall octane numbers are calculated by taking the average of the research and motor number. Toluene is known for having an octane number of 114, much higher than regular gasoline at 84 octane and premium at 93 octane. This means it is high energy burning fuel and reduces knocking in heavily loaded engines. High performance racing cars require large amounts of toluene in their fuel, due to the extreme load these engines undergo. The toluene-benzene product is a good waste-derived alternative to traditional racing fuels and is desirable by sponsors and racing organizations for it being an alternative to fossil fuels (“Toluene - Additive for...” 2014). For diesel fuel, studies have been conducted showing the addition of toluene to diesel decreases carbon monoxide emissions, allowing for more complete combustion of fuel inside the engine (Özer 2020). Ultimately, the product stream provides good potential for the alternative fuels market.

The second product separated from the process is recycled ethylbenzene at 85% purity by weight diluted with xylene from the top of T-102. Ethylbenzene is commonly used as a feedstock to create styrene and ultimately polystyrene plastic. However, at 85% purity, it would be uneconomical to upcycle this material to compete with virgin ethylbenzene, therefore, it is more suited for use in synthetic rubber, ink, or solvents (United States and Taylor 2010). Styrene is the next product separated out of the process, coming off the top of T-103. This follows a similar

trend to ethylbenzene, only coming out at 83% purity by weight. Styrene's main use is in the production of polystyrene, the plastic that the pyrolysis oil used in the separation is derived from. Again, the low purity of the component makes it uncompetitive for the recycled plastic monomers market. Higher purity components could be achieved with larger distillation tower designs; however, the low cost of virgin plastic monomer feedstock makes additional investment in this equipment uneconomical.

The final product separated from the process is cumene, coming out in small amounts off the bottom of T-103 at 95% purity by weight. This higher purity could make it more competitive than crude oil cumene, however, it is only produced at 173 kg/h from the process, nowhere near enough material to justify the cost of the process. Cumene is primarily used in the production of phenol and as an additive to aviation fuel or acetone. The cumene produced here would be an excellent source of waste derived aviation fuel. Unfortunately, North American demand for cumene is expected to decline, questioning the profitability of separating this component out of the process in the first place ("Cumene" 2022).

The minimum product break even prices, as shown in Table 14, are lower than the average market prices for the pure monomers, however, the products being sold are significantly less pure. The product prices can be competitive if customers can sufficiently use these products in their processes because they can access them for cheaper prices than those of the pure monomers. A viable option for this plant may be to make an agreement with a customer to be the sole supplier of one of these products at the cheaper price point.

The effect of pressure on the second and third distillation columns also affects the overall profitability of the system. To draw a vacuum in the column, steam ejector loads were estimated which contributes to the overall yearly utility cost. The reduction in pressure also decreases the

overall column size by decreasing the number of trays needed to achieve the desired product cuts. In T-102, the lowered purchase cost of the column was significant enough to offset the increased utility required to pull a vacuum of 0.1 bar, making the lower operating pressure the more cost-effective option.

Another option to improve the profitability of the system is to remove T-102 and T-103 from the process relying on one product stream of revenue. With the removal of the second two towers in the process, the remaining aromatic mix would make a viable feedstock for separation in a refinery into fuel feedstock. All the components present in the feed and products of this process exist within the existing oil refining technology chain, meaning the ability to sell these products directly into the refining ecosystem could be viable. Also, if the goal is to use this mix as a fuel additive, this process could be implemented as an addition to an existing refinery, potentially repurposing existing equipment to further reduce the capital cost. This can allow refineries to boost octane ratings of gasoline using a cheap feedstock. It is recommended to investigate the addition of this equipment into existing refining structures.

Due to the temperature sensitive nature of the monomer components in the process, keeping the process temperature within a safe specified range is of utmost importance as excessive fouling could result in process downtime. The most likely place to find these high temperature zones would be in the reboiler sections of the distillation towers and the lower trays. Focusing on these hot spots, preventative measures can be used to minimize the fouling effect. For tower reboilers, there are two choices. The first is a traditional kettle reboiler, which involves a large vessel that has a controlled liquid level and a high vapor percentage heading back into the tower. The benefit of this design is it is easy to service and efficient at near vacuum pressures. The disadvantages are that it requires a high capital investment due to the large vessel size.

Additionally, kettle reboilers operate at a lower circulation rate, meaning they are highly susceptible to fouling (Pourazimi 2020).

The second choice for a reboiler design is either a horizontal or vertical thermosyphon reboiler. Vertical thermosyphon reboilers are good at minimizing fouling due to high circulation rate; however, they are much harder to service due to their vertical nature. A horizontal thermosyphon reboiler provides less fouling resistance than a vertical; however, the cost to service is much lower due to its orientation, provided there is sufficient space in the plant design (Pourazimi 2020). Horizontal thermosyphon reboilers are thus chosen for all towers in this design. The reasoning is due to the need to minimize fouling while also minimizing costly plant downtime. Therefore, the design calls for investment in spare reboilers, due to the ability to service them independent of tower operation. This takes advantage of the low area and utility cost already captured due to the vacuum conditions.

When it comes to trays, a preventative approach to reducing fouling is crucial due to the high cost of maintenance for distillation columns if the trays were to become extremely fouled. Any moving valve tray is a poor choice, even though moving valve trays allow for better liquid-vapor contact over different vapor velocities, due to the movement of the valves becoming inoperable with fouling. Fixed valve trays are the optimal choice to prevent tray fouling. Sieve trays were chosen due to their fixed valve design and their economic advantages (Herbert et al. 2016).

Even with preventative measures to prevent polymer formation and fouling, a complete design requires mitigative measures as well. Even with preventative measures, the risk of a runaway polymerization reaction exists, especially in the reboiler sections where the process temperature reaches levels close to spontaneous polymerization. A layer of protection analysis

(LOPA) of a polymerization reaction in a reboiler is explored in Table 15 below. The scenario analysis explores an over-pressure of a reboiler vessel from an external fire that raises the process temperature to a level creating a runaway polymerization of either styrene or ethylbenzene. Over pressuring could also be potentially caused by loss of utility to the steam ejector, causing a rapid pressure increase resulting in temperature increase of the system resulting in polymerization. As a result of the LOPA, it is recommended to include pressure relief valves in all reboilers, distillation columns, and heat exchanger vessels to prevent such events. Additionally, safety instrumented systems for the whole plant are required to safely stop the process to avoid runaway reactions affecting multiple equipment.

Table 15: Layers of protection analysis of a scenario involving a runaway reaction in a reboiler.

LOPA Worksheet	
Description of Event	Reboiler of tower T-101 becomes over pressured due to runaway polymerization reaction as a result of an external fire
1. Initiating Event (Cause) - Table 12-2	Large External fire
2. Severity Level	Very serious, overpressure could result in explosion with a likely fatality and release of carcinogenic and flammable material
3. Likelihood	1E-2
4. Risk Level	B
5. Target mitigated event frequency (TMEF)	1E-5
6. Enabling Conditions	1
7. Conditional Modifiers	none
8. Adjusted IE Frequency (Multiply 1*6*7)	1E-2
9. Existing layers of protection	none
10. Frequency with existing layers of protection	1E-2
11. Additional layers of protection required	1E-3, (pressure safety valve 1E-2, and safety instrumented system 1E-1)

The chemical components undergoing the proposed process are considered flammable hydrocarbons. Extra precautions should be taken in the event of a release to avoid ignition. All

chemicals are irritating to human skin and personnel should avoid contact with all liquids and vapors. Benzene is a component in the toluene fuel additive and is a known carcinogen. All products in the process are considered to have trace benzene and therefore use of the component needs to follow all regulatory requirements. Cumene, xylene, ethylbenzene, and styrene are toxic in large quantities. It is recommended that proper personal protective equipment should always be worn for individuals in proximity to the process and personnel should avoid contact at all costs. Access to detailed chemical safety information for each component is included in Appendix C.

A major risk associated with vacuum systems, as with other pressure vessels, is the vessel rating and ability to resist buckling. The thickness of the vessel shell should be sized to fit the operating pressure and be able to withstand pressure testing prior to start up. If vacuum is lost, and pressure begins to build in the vessel, pressure relief devices should be installed to vent to flare to prevent a release of flammable material to atmosphere. A concern unique to vacuum distillation in hydrocarbons is the risk of a leak in the vessel wall, pipes, or welds. Unlike vessels operating at or above ambient pressure, a leak in the system would pull air into the distillation column, creating a flammable environment due to the introduction of oxygen. This creates the risk of fire and explosion in the distillation column. The pressure of the vessel should be monitored closely for any gradual increases that would indicate an air leak, and the vessel should be equipped with an oxygen detection system.

The pyrolysis oil involved in this process is entirely composed of aromatic hydrocarbons. The distillation of hydrocarbon material demands strict process safety design. When hydrocarbon liquids are distilled, they are vaporized and in their flammability range, resulting in possible explosions and fires in distillation related equipment. Rigorous operator training, pre-emergency

planning, and management of change processes are all managerial controls that should be utilized to prevent accidents. Additionally, plant design can help prevent exacerbating accidents when they occur by spacing out high risk equipment, which in the process proposed here, would be the reboilers of each column (“Distillation of flammable...”). Pressure relief valves are essential in mitigating possible overpressure events which could lead to a fire or explosion. All pressure relief valve outlets and excess overhead gases should be vented to a flare for atmospheric combustion. For this process design, overpressure events could originate from vessel and pipe leaks, loss of cooling or heating utility, loss of vacuum utility, or external fires affecting vessel temperature. Additional mitigative measures should include fire retardant systems such as fire extinguishers and water towers to assist in preventing fire spread (“Distillation of flammable...”). It is recommended to utilize managerial controls and smart plant design to reduce employee risk. It is also recommended to implement preventative and mitigative measures such as pressure relief valves, temperature and level control loops, and safety instrumented systems in the process.

Environmental stewardship stands as a pillar of the chemical engineering code of ethics. The components involved with this process are toxic and flammable, meaning their release to the environment should be avoided whenever possible. A flare is used to completely combust excess gas and air from the process, breaking down the toxic substances into carbon dioxide and water. Table 16 below describes the recordable quantity thresholds for each component used in the process in the incident of a release into the environment. Areas in the process that should be closely monitored for environmental releases are any loading and unloading of feed and products, any flaring event, and startups and shutdowns. It is recommended to monitor and prevent all environmental releases if possible.

Table 16: Recordable quantity thresholds regulated by the United States Environmental Protection Agency.

Component	Recordable Quantity (lbs)
Benzene	10
Toluene	1000
Ethylbenzene	1000
Xylene	100
Styrene	1000
Cumene	5000

Literature Cited

- “Cumene.” *Chemical Economics Handbook*, S&P Global, June 2022, <https://www.spglobal.com/commodityinsights/en/ci/products/cumene-chemical-economics-handbook.html>.
- “Distillation of Flammable or Combustible Liquids.” *Property Risk Consulting Guidelines*, AXA XL Risk Consulting, <https://axaxl.com/-/media/axaxl/files/pdfs/prc-guidelines/prc-9/prc9621distillationofflammableorcombustibleliquidsv1.pdf>.
- Geyer, Roland, et al. “Production, Use, and Fate of All Plastics Ever Made.” *Science Advances*, vol. 3, no. 7, 19 July 2017, <https://doi.org/10.1126/sciadv.1700782>.
- Herbert, Scott, and Neil Stanford. “Consider Moving to Fixed Valves.” *AICHE*, American Institute of Chemical Engineers, 9 May 2016, <https://www.aiche.org/resources/publications/cep/2016/may/consider-moving-fixed-valves>.
- Özer, Salih. (2020). The effect of adding toluene to increase the combustion efficiency of biodiesel. *Energy Sources Part A Recovery Utilization and Environmental Effects*. 42. 1-17. 10.1080/15567036.2020.1776421.
- Pourazimi, Sina. “Reboiler Selection Essentials.” *Process Phase*, 31 Dec. 2020, <https://processphase.com/reboiler-selection-essentials/>.
- Qureshi, Muhammad Saad, et al. “Pyrolysis of Plastic Waste: Opportunities and Challenges.” *Journal of Analytical and Applied Pyrolysis*, vol. 152, Nov. 2020, <https://doi.org/https://doi.org/10.1016/j.jaap.2020.104804>.
- Reusch, William. “Polymers.” *MSU Chemistry*, 5 May 2013, <https://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/polymers.htm>.
- “Toluene - Additive for Racing Fuels, Fuel Octane Booster.” *Worldofchemicals.com*, World of Chemicals, 25 Jan. 2014, <https://www.worldofchemicals.com/428/chemistry-articles/toluene-additive-for-racing-fuels-fuel-octane-booster.html>.
- Tullo, Alexander. “Amid Controversy, Industry Goes All in on Plastics Pyrolysis.” *Chemical & Engineering News*, American Chemical Society, 10 Sept. 2022, <https://cen.acs.org/environment/recycling/Amid-controversy-industry-goes-plastics-pyrolysis/100/i36>.
- Turton, Richard, et al. *Analysis, Synthesis, and Design of Chemical Processes*. 5th ed., Pearson Education, Inc., 2018.
- “Typical Data Polyflow Pygas.” 20 Mar. 2009.

United States, Congress, Agency for Toxic Substances and Disease Registry, and Jessilyn Taylor. *Toxicological Profile for Ethylbenzene*, U.S. Dept. of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry, 2010.

Zhao, Lin, et al. "Probing into Styrene Polymerization Runaway Hazards: Effects of the ..."
Probing into Styrene Polymerization Runaway Hazards: Effects of the Monomer Mass Fraction, ACS Publications, 3 May 2019,
<https://pubs.acs.org/doi/10.1021/acsomega.9b00004>.

Appendix A: Project Data

Table A.1: Relative volatility data for components in pyrolysis oil feed stream using Antoine's equation at 1 bar and 125°C, the bubble point of the feed.

Component	mole% in feed	weight% in feed	T (K)	A	B	C	P* (bar)	Ki (1 bar)	Kixi	Relative Volatility	
Benzene	6.15	4.77	398.2	4.6	1660.7	-1.5	2.44	2.44	0.15		
Toluene	27.69	25.35	398.2	4.5	1738.1	0.4	1.53	1.53	0.42	Tol- Ben	1.60
Ethylbenzene	24.61	25.96	398.2	4.1	1419.3	-60.5	0.74	0.74	0.18	EB- Tol	2.05
Xylene	9.24	9.75	398.2	4.1	1463.2	-58.0	0.68	0.68	0.06	Xyl- EB	1.09
Styrene	27.69	28.65	398.2	4.2	1525.1	-56.4	0.57	0.57	0.16	Sty- Xyl	1.19
Cumene	4.62	5.52	398.2	4.1	1455.8	-65.9	0.47	0.47	0.02	Cum- Sty	1.22

Table A.2: Relative volatility data for components in pyrolysis oil feed stream using Antoine's equation at 0.5 bar and 102°C, the bubble point of the feed.

Component	mole% in feed	weight% in feed	T (K)	A	B	C	P* (bar)	Ki (1 bar)	Kixi	Relative Volatility	
Benzene	6.15	4.77	329.9	4.6	1660.7	-1.5	0.33	3.28	0.2		
Toluene	27.69	25.35	329.9	4.1	1346.4	-53.5	0.16	1.63	0.45	Tol- Ben	1.71
Ethylbenzene	24.61	25.96	329.9	4.1	1419.3	-60.5	0.06	0.64	0.16	EB- Tol	2.16
Xylene	9.24	9.75	329.9	4.1	1463.2	-58.0	0.06	0.57	0.05	Xyl- EB	1.10
Styrene	27.69	28.65	329.9	4.2	1525.1	-56.4	0.04	0.44	0.12	Sty- Xyl	1.22
Cumene	4.62	5.52	329.9	4.1	1455.8	-65.9	0.03	0.35	0.02	Cum- Sty	1.23

Table A.3. Relative volatility data for components in pyrolysis oil feed stream using Antoine's equation at 0.1 bar and 56.8°C, the bubble point of the feed.

Component	mole% in feed	weight% in feed	T (K)	A	B	C	P* (bar)	Ki (1 bar)	Kixi	Relative Volatility	
Benzene	6.15	4.77	329.9	4.6	1660.7	-1.5	0.33	3.28	0.2		
Toluene	27.69	25.35	329.9	4.1	1346.4	-53.5	0.16	1.63	0.45	Tol- Ben	2.02
Ethylbenzene	24.61	25.96	329.9	4.1	1419.3	-60.5	0.06	0.64	0.16	EB- Tol	2.54
Xylene	9.24	9.75	329.9	4.1	1463.2	-58.0	0.06	0.57	0.05	Xyl- EB	1.12
Styrene	27.69	28.65	329.9	4.2	1525.1	-56.4	0.04	0.44	0.12	Sty- Xyl	1.29
Cumene	4.62	5.52	329.9	4.1	1455.8	-65.9	0.03	0.35	0.02	Cum- Sty	1.27

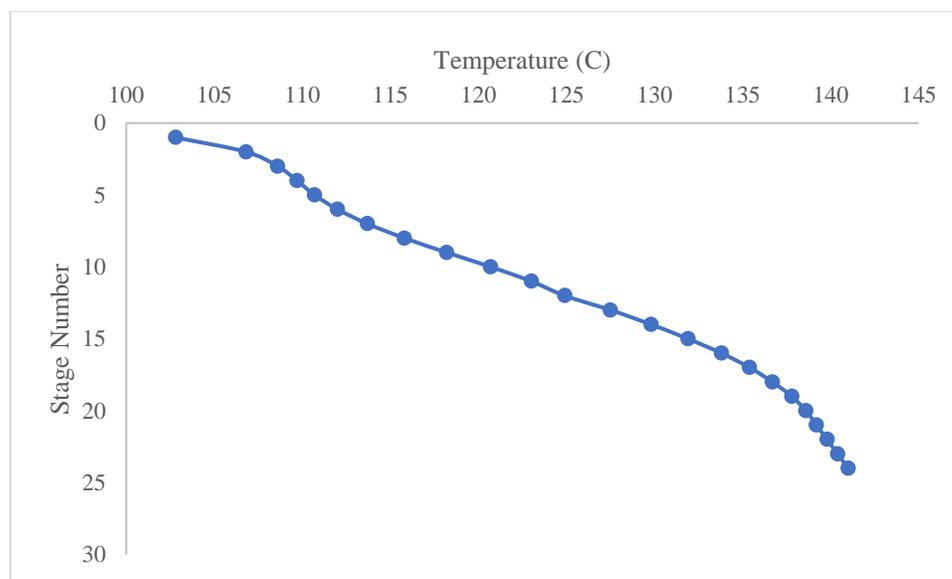


Figure A.1. The temperature profile for T-101 with the feed at tray 12 and the total number of 22 trays.

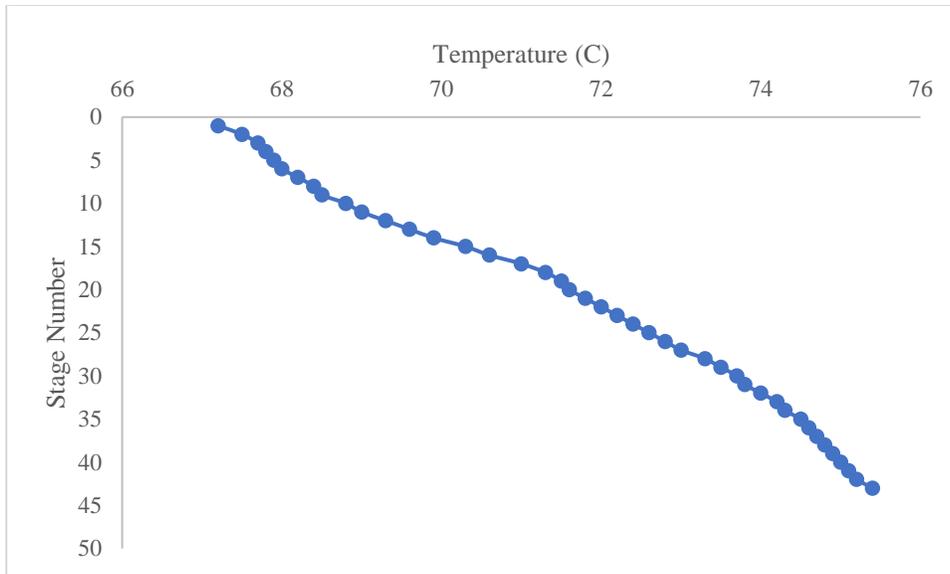


Figure A.2. Temperature profile for T-102 with the feed at tray 18 and the total number of 41 trays.

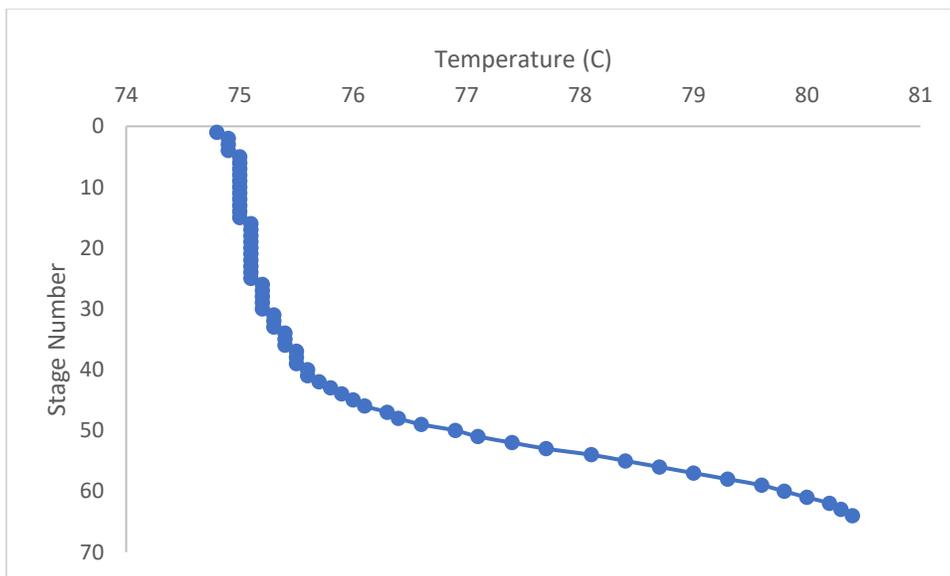


Figure A.3. Temperature profile for T-103 with the feed at tray 34 and the total number of 62 trays.

Appendix B: Sample Calculations

Antoine Equation:

1. $\log_{10}P = A - B/(T + C)$ where P = vapor pressure (bar), T = Temperature (K)

Relative Volatility:

2. $\frac{K_1}{K_2} = \alpha$ where K = vapor pressure/ pressure

Overall Heat Transfer:

3. $Q = U \times A \times \Delta T_{lm}$ where Q = heat transferred (W), U = Overall heat transfer coefficient (W/m²-K), A = heat transfer area (m²)

4. $\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln \left(\frac{\Delta T_1}{\Delta T_2} \right)}$ where ΔT_1 = temperature differential between warm streams (K), and ΔT_2 = temperature differential between cold streams (K)

Steam Injector Sizing:

5. $m_{air-leak} = CV^{2/3}$ where V = volume of process vessel (m³) and C = is a coefficient based on vacuum pressure in Table 23.17 (Turton et al. 2018) (kg/m²/h)

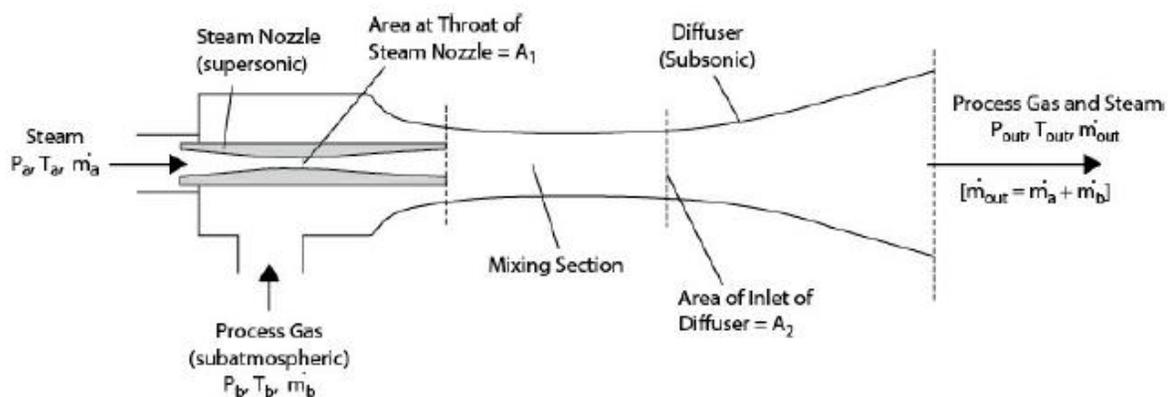


Figure 23.15 Diagram of the Processes and Notation Used in the Design of a Single-Stage Steam Ejector

Imaged sourced from page 1073 (Turton et al. 2018).

6. $\left[\frac{m_b}{m_a}\right]_2 = \left[\frac{m_b}{m_a}\right]_1 \sqrt{\left(\frac{M_b}{M_a}\right)_2 \left(\frac{T_a}{T_b}\right)_2}$ Where m_b/m_a is the entrainment ratio derivable from an ideal case using figures 23.16 and 23.17 for an ideal case. Refer to figure 23.15 above for a visual representation of the relationship. M_a and M_b are the molar masses of each steam and the process gas.

Grassroots Costing:

7. $C_p^o = 10^{K_1 + K_2 * \log A + K_3 * (\log A)^2}$
8. $C_{BM} = C_p^o (B_1 + B_2 F_M F_P)$
9. $C_{TM} = C_{BM} * 1.18$
10. $C_{GR} = C_{TM} + 0.5 C_{BM}$

EAOC:

11. $EAOC = -(\text{product value} - \text{feed cost} - \text{utility costs} - \text{waste treatment costs} - \text{capital cost annuity})$
12. $\text{capital cost annuity} = FCI * \frac{i(1+i)^n}{(1+i)^{n+1}}$

Labor Costing:

13. $N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5}$

Appendix C: Chemical Safety Information

Cumene:

<https://cameochemicals.noaa.gov/chemical/3018#:~:text=A%20clear%20colorless%20liquid%20with,Vapors%20heavier%20than%20air.>

Toluene:

<https://cameochemicals.noaa.gov/chemical/4654#:~:text=Highly%20flammable.,Insoluble%20in%20water.&text=TOLUENE%20reacts%20vigorously%20with%20allyl,reported%20%5BNFP%20A%20491M%201991%5D.>

Styrene:

<https://cameochemicals.noaa.gov/chemical/4553#:~:text=STYRENE%20MONOMER%20is%20a%20colorless,%2C%20J.%2C%20Loss%20Prev.>

Benzene:

<https://cameochemicals.noaa.gov/chemical/2577#:~:text=potentially%20incompatible%20absorbents.-,The%20information%20in%20CAMEO%20Chemicals%20comes%20from%20a%20variety%20of,Slightly%20soluble%20in%20water.&text=BENZENE%20reacts%20vigorously%20with%20allyl,dichloride%20or%20ethyl%20aluminum%20sesquichloride.>

Xylene:

<https://cameochemicals.noaa.gov/chemical/8151#:~:text=A%20clear%20colorless%20liquid%20with,water%20and%20insoluble%20in%20water.>

Ethylbenzene:

[https://cameochemicals.noaa.gov/chemical/6424#:~:text=A%20clear%20colorless%20liquid%20with,gal\)%20and%20insoluble%20in%20water.](https://cameochemicals.noaa.gov/chemical/6424#:~:text=A%20clear%20colorless%20liquid%20with,gal)%20and%20insoluble%20in%20water.)

Appendix D: Project Files

[Project Costing](#)

[Component Info](#)

ChemCAD file available upon request