Spring 5-7-2022

Optimization of an Ethylbenzene to Styrene Production Facility

John Michels

Recommended Citation

Michels, John, "Optimization of an Ethylbenzene to Styrene Production Facility" (2022). *Honors Theses*. 2622.
https://egrove.olemiss.edu/hon_thesis/2622

OPTIMIZATION OF AN ETHYLBENZENE-TO-STYRENE PRODUCTION FACILITY

by

John Curtis Michels, Hollie Arnsdorff, Victoria Hunter

A thesis submitted to the faculty of the University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College

Oxford

May 2022

Approved By

Advisor: Dr. Adam Smith

Carroll

Reader: Professor David Carroll

Joanna Harrelson

Reader: Professor Joanna Harrelson

ACKNOWLEDGEMENTS

I would like to acknowledge my teammates for this project, Hollie Arnsdorff and Victoria Hunter. Their contributions towards both optimization and simulation portions of this project, in addition to their outstanding leadership, were key to the success of this project. I would like to also to thank Mike Gill, David Carroll, Adam Smith, Joanna Harrelson, and the rest of the faculty of the University of Mississippi’s Department of Chemical Engineering for their support and insight.

ABSTRACT

JOHN CURIS MICHELS: Optimization of an Ethylbenzene-to-Styrene Production Facility

(Under the direction of Adam Smith)

The purpose of this case study is to optimize the design and production of an ethylbenzene-to-styrene manufacturing facility, Unit 500. Compared to the original base-case design, the optimizations presented in this document will save approximately $337 million dollars without compromising the production requirements or quality. Optimization of this process used net present value as an objective function, with changes centered around the reactors, but also the separation equipment and exchangers prior to separation, as those devices most directly controlled process stream contents and conditions. The second set of reactors was removed in favor of using one optimized set of reactors, in addition to decreasing the three-phase separators temperature and modifying both the number of trays and the material of construction for the distillation towers. A utilities and exchangers analysis was performed, but the course of action found from it was deemed unrecommended due to excess complexity of the new model. Separately, an isothermal styrene reactor was optimized for 5% minimum conversion utilizing PRO/II, and found that

A more detailed market analysis and a second optimization cycle is recommended before making a firm decision if building the facility to produce styrene would be preferred to purchasing it from the open market, but current market conditions suggest that manufacturers of styrene are more likely to use it to produce higher-value products rather than selling it in bulk. In this case, securing a styrene vendor is unlikely and making the styrene will be preferred, as the value from producing polystyrene later in the process will offset the losses in Unit 500.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

TABLE OF ABBREVIATIONS

AE	Annual equivalent
barg	Bar pressure (gauge)
C	Celsius
CW	Cooling water
FCI	Fixed capital investment
HPS	High pressure steam
hr	Hour
K	Kelvin
Kmol	Kilomoles
kPa	Kilopascals
L/D	Length-to-diameter ratio
LPS	Low pressure steam
m	Meters
m^3	Cubic Meters
NPV	Net present value

BASE CASE SUMMARY

The proposed styrene production process was designed to operate 8,000 hours per year and produce 100,000 tonnes per year of 99.8% by weight styrene via the dehydrogenation of ethylbenzene. The ethylbenzene feed stream is 98% by mole ethylbenzene, 1% benzene, and 1% toluene. This feed stream then mixes with an ethylbenzene recycle stream before being heated by the feed heat exchanger E-501 with high-pressure steam as its utility. This stream then mixes with superheated steam to increase the temperature of the process stream before entering the endothermic reactor series. The packed bed adiabatic reactor was set with the following reaction system, which can be found in Appendix B of Turton et al[1]:

$$C_6H_5C_2H_5 \rightleftharpoons C_6H_5C_2H_3 + H_2 \qquad r_1 = 6.2exp(-90,981/RT)p_{eb} \quad \text{(forward)}$$

$$r_2 = 6x10^{-5}exp(-61,12/RT)p_{sty}p_{H2} \quad \text{(reverse)}$$

$$C_6H_5C_2H_5 \rightarrow C_6H_6 + C_2H_4 \qquad r_3 = 2.71x10^{7}exp(-207,98/RT)p_{eb}$$

$$C_6H_5C_2H_5 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \qquad r_4 = 6.45x10^{-4}exp(-91,51/RT)p_{eb}p_{H2}$$

***Equations 1-3**: Reaction Mechanism Equations.*

Where p_i is the partial pressure of the respective component in pascals (Pa), T is the temperature in Kelvin (K), the activation energy is in joules per mole, and the rate is in moles per m^3 catalyst per second. R-501a-e was modeled as five packed bed reactors. Equation 1, the reaction of ethylbenzene to styrene and hydrogen, contains two reaction rate equations due to its reversibility. Equation 2 shows the conversion of ethylbenzene to benzene and ethylene, and Equation 3 shows the conversion of ethylbenzene and hydrogen to toluene and methane. More details regarding the reaction itself can be found in Appendix B of Turton et al[1].

The reactor effluent from R-501a-e was then sent to E-502 where it was heated using the remaining superheated steam from H-501. The process stream then enters the second reactor series R-502 a-e, which was modeled as a set of five adiabatic packed bed reactors in parallel. The superheated steam is generated by heating low pressure steam using a steam heater, H-501. The superheated steam leaving the heater then splits, with part going to heat the ethylbenzene stream and part going to the utility side of exchanger E-502.

The reactor effluent is then cooled by three heat exchangers in series. The first heat exchanger, E-503 uses a condensing high pressure stream. The stream is then cooled in E-504 which utilizes condensing low-pressure steam. Finally, cooling water in E-505 cools the stream. The process stream is then separated in a three-phase separator, V-501. The vapor phase leaves from the top of the vessel where a valve is then used to adjust the pressure. The liquid water phase leaves from the bottom of V-501 where the pressure is then increased in P-501 before leaving the process as wastewater.

The liquid organic phase leaves from the middle of the vessel and is sent to a Benzene/Toluene Column, T-501. This column has a total reboiler and a partial condenser. The vapor component of the distillate leaves the reflux drum from the top and mixes with the vapor component of the three-phase separator. This stream is then compressed in C-501 before leaving the process as fuel gas. The liquid component of the distillate is pressurized in pump P-504 and then leaves the process as a benzene/toluene product stream. The bottoms of T-501 require further separation and are sent to a styrene column, T-502 to purify the styrene product. This column has a total condenser and reboiler. The distillate stream, or ethylbenzene recycle, is pressurized in P-506 before mixing with the ethylbenzene feed stream. The bottoms of T-502 are pressurized in P-505 before leaving the process as the styrene production stream.

BASE CASE PROCESS FLOW DIAGRAM

Styrene from Ethylbenzene: Base Case Process Flow Diagram

Heat Exchangers	
E-501 Feed Heater	E-506 Reboiler
E-502 Inter-heater	E-507 Condenser
E-503 Product Cooler	E-508 Reboiler
E-504 Product Cooler	E-509 Condenser
E-505 Product Cooler	

Pumps & Compressors	
P-501 A/B Wastewater Pump	P-506 A/B Recycle Pump
P-502 A/B Reflux Pump	C-501 Fuel Gas Compressor
P-503 A/B Reflux Pump	
P-504 A/B Benzene/Toluene Pump	
P-505 A/B Styrene Pump	

Vessels	
V-501 3-Phase Separator	V-503 Reflux Drum
V-502 Reflux Drum	

Towers	
T-501 Benzene/Toluene Column	T-502 Styrene Column

Reactors	
R-501 a-e Ethylbenzene to Styrene Reactors	R-502 a-e Ethylbenzene to Styrene Reactors

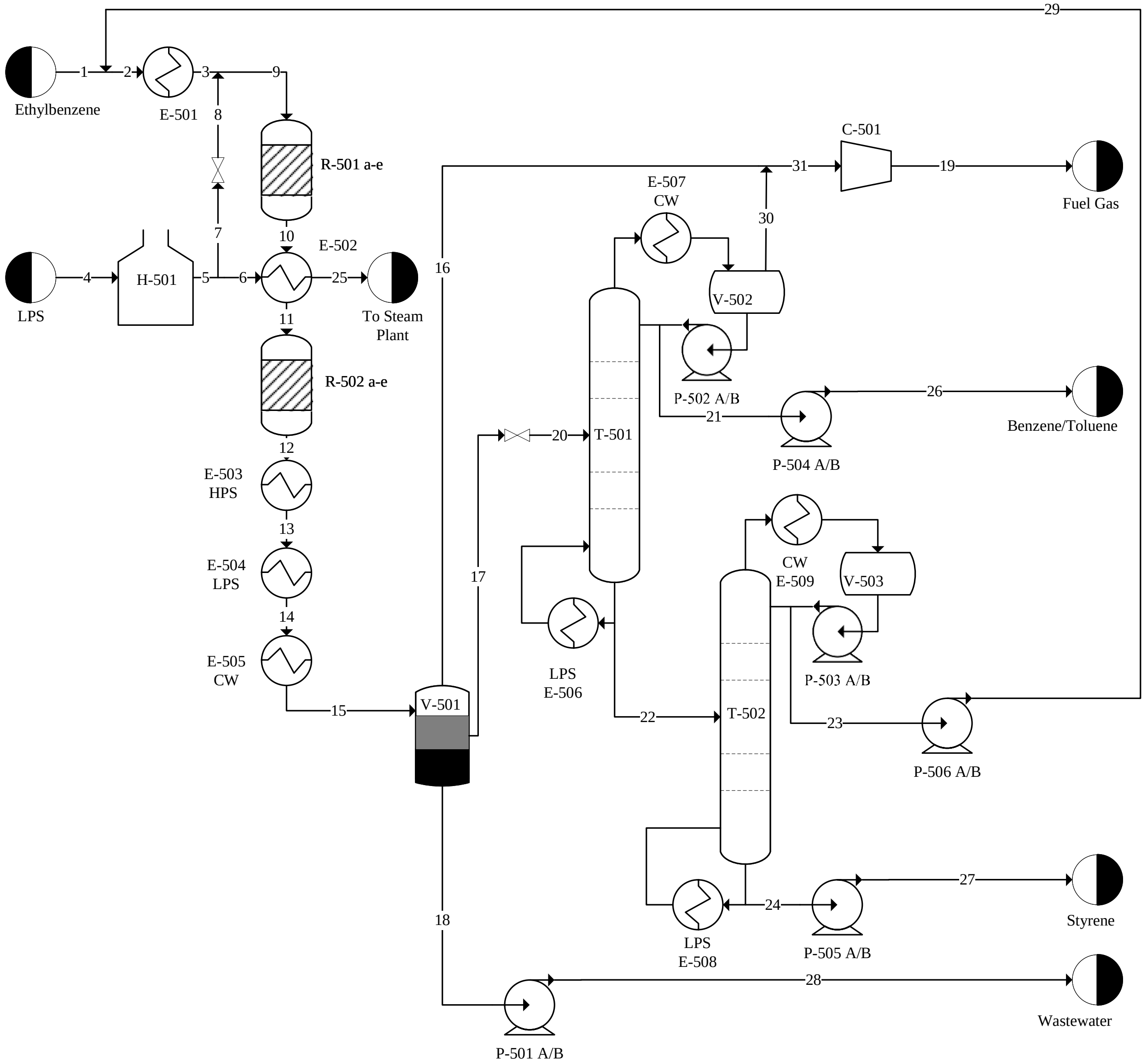

Figure 1: *Base Case Process Flow Diagram*

BASE CASE ECONOMIC MODEL

The economic model for the base case was prepared in advance for this project using pricing indices and methods from Turton et al[1]. Each piece of equipment from the base case was individually priced by utilizing Turton's price approximations found in Appendix A of the text[1], considering cost of material, size and expected performance. Each piece of equipment, while following a 2015 pricing index, had its price adjusted to follow expected inflation rates from 2015 to 2021 to provide an accurate cost of equipment. Accounting for land and fixed capital investment, which covers labor costs for construction and the price of startup raw materials, the grassroots facility cost was approximated.

The approximated cost of various aspects of operation for this facility, including raw materials, utilities, and labor, were estimated for each year of operation, and adjusted for the value of money decreasing over time. Taking into account total costs, revenue and depreciation, the net present value (NPV) was found for this project. The annual equivalent (AE) was also calculated to serve as a measure for expected yearly cost for running and maintaining the facility, and the fixed capital investment (FCI) was estimated as an initial cost for construction of the facility and the purchase of materials and labor for initial operation. The key metrics in the base case economic model are summarized below:

Table 1: *Summary of Base Case Metrics*

Net Present Value ($M)	Annual Equivalent ($M)	Fixed Capital Investment ($M)
-863	-139	-205

It is important to note that the styrene produced by the plant is intended to be used internally, as this facility's status as Unit 500 implies other Units being connected towards this one. The NPV discussed throughout this report treats styrene as if it is being sold. Doing so enables a clear comparison of the price difference in making the styrene as compared to buying the styrene. A positive NPV means that it would be cheaper to make the styrene than to buy the styrene, a zero NPV means that the cost of making styrene is equal to the price of buying styrene, and a negative NPV means that it would be cheaper to buy the styrene than to make the styrene.

OPTIMIZATION SUMMARY

The process of optimizing the base case focused on increasing the NPV of the project by changing various aspects of the equipment. One optimization cycle was used for each value that was adjusted, with multiple data points used per value optimized. The adjusted values for this project include: number of reactors, pre-heated steam flow (this controlled reactor temperature), reactor pressure, reactor volume, distillation column conditions, and number of exchanger/utilities.

Upon the removal of the second set of reactors, R-501 a-e had to be re-designed to fit the same production standards as the original set reactors in the base case. The number of reactors was optimized to be set to 11 as compared to the original total of 10 reactors with 5 per reactor set (R-501 a-e and R-502 a-e), and the new length-to-diameter ratio was found to be optimal when reactor diameter is half the value of the reactor length, the minimum recommended for typical reactor construction. The optimized pressure for R-501A-K was found to be approximately 240 kilopascals, as increasing the pressure further than this was starting to move close to the safety design limit for a typical reactor, and lower pressures found reduced NPV over higher pressure. Steam flow rate was found to best fit the process at 8500 kilogram-moles per hour. The three-phase separator was found to have an optimal operation pressure of 185 kilopascals and a feed temperature of 25 Celsius, resulting in further increase in NPV accounting for changes to exchanger utility changes. The off-gas compressor was substituted with two smaller compressors to fit recommended operation parameters, and an intercooler was added between them to ensure product temperature is the same as before. Adjustments to the purity of non-product streams for both distillation towers in addition to the change in tower construction material from titanium to carbon steel allowed for further optimization of the NPV, with a final project NPV of -$525 million.

OPTIMIZED PROCESS FLOW DIAGRAM

Styrene from Ethylbenzene: Optimized Process Flow Diagram

Heat Exchangers	
E-501 Feed Heater	E-506 Reboiler
E-503 Product Cooler	E-507 Condenser
E-504 Product Cooler	E-508 Reboiler
E-505 Product Cooler	E-509 Condenser

Pumps & Compressors	
P-501 A/B Wastewater Pump	P-506 A/B Recycle Pump
P-502 A/B Reflux Pump	C-501 Fuel Gas Compressor
P-503 A/B Reflux Pump	C-502 Fuel Gas Compressor
P-504 A/B Benzene/Toluene Pump	
P-505 A/B Styrene Pump	

Vessels	
V-501 3-Phase Separator	V-503 Reflux Drum
V-502 Reflux Drum	

Towers	
T-501 Benzene/Toluene Column	T-502 Styrene Column

Reactors
R-501a-k Ethylbenzene to Styrene Reactors

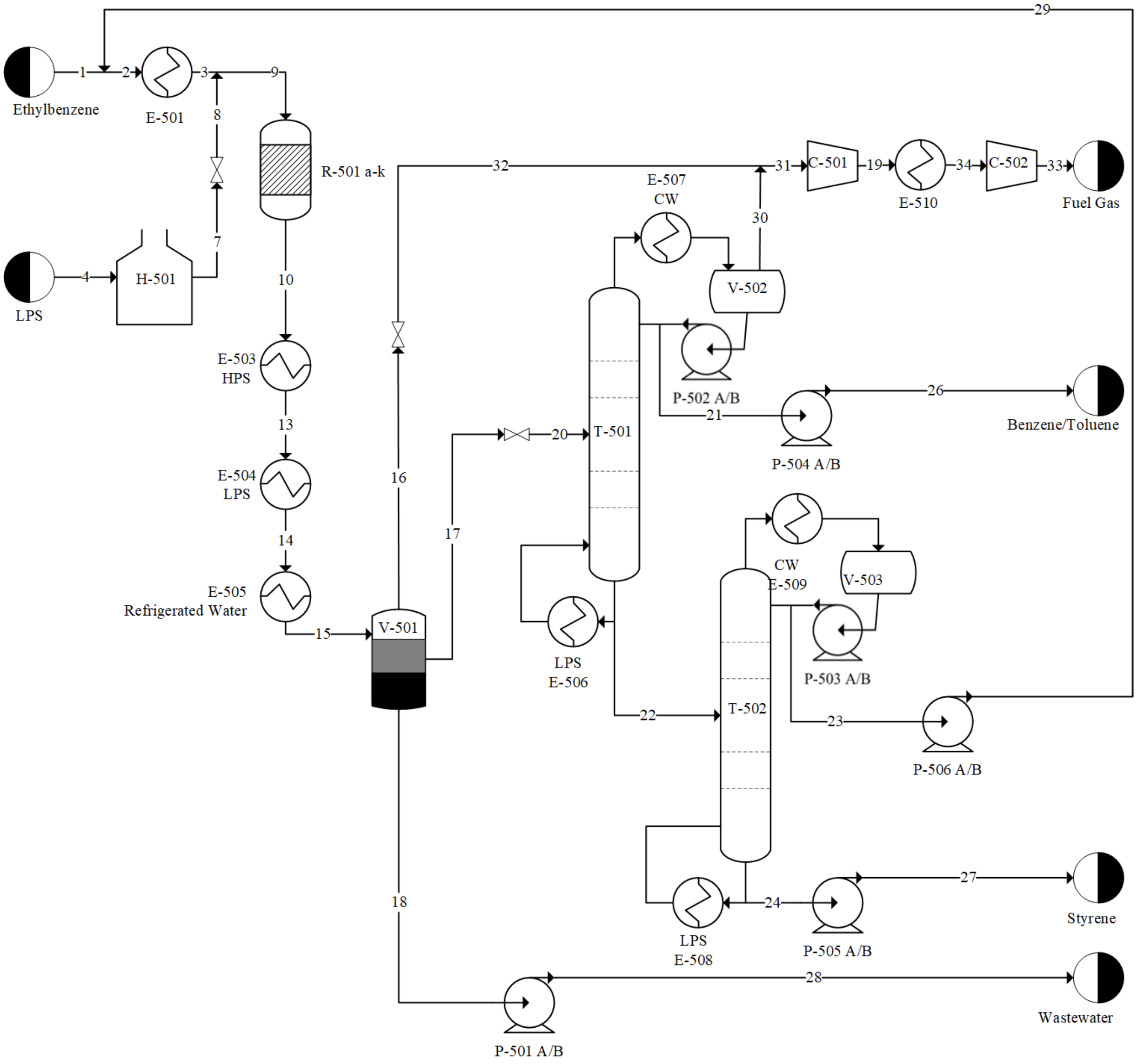

Figure 2: *Optimized Process Flow Diagram*

OPTIMIZATION DESCRIPTION

The first step taken in the optimization of the styrene production process was the removal of the second series of reactors, R-502 a-e, and the corresponding heat exchanger, E-502. Due to the significant decrease in reactor volume available, the NPV decreased greatly upon the removal of the reactors. This immediate change in NPV was not a good indicator of whether or not there was a benefit in the removal of R-502 a-e until the new reactor conditions were updated. The number of reactors in the R-501 series was optimized, and the results of this optimization indicated whether or not removing R-502 a-e would be a wise economic decision.

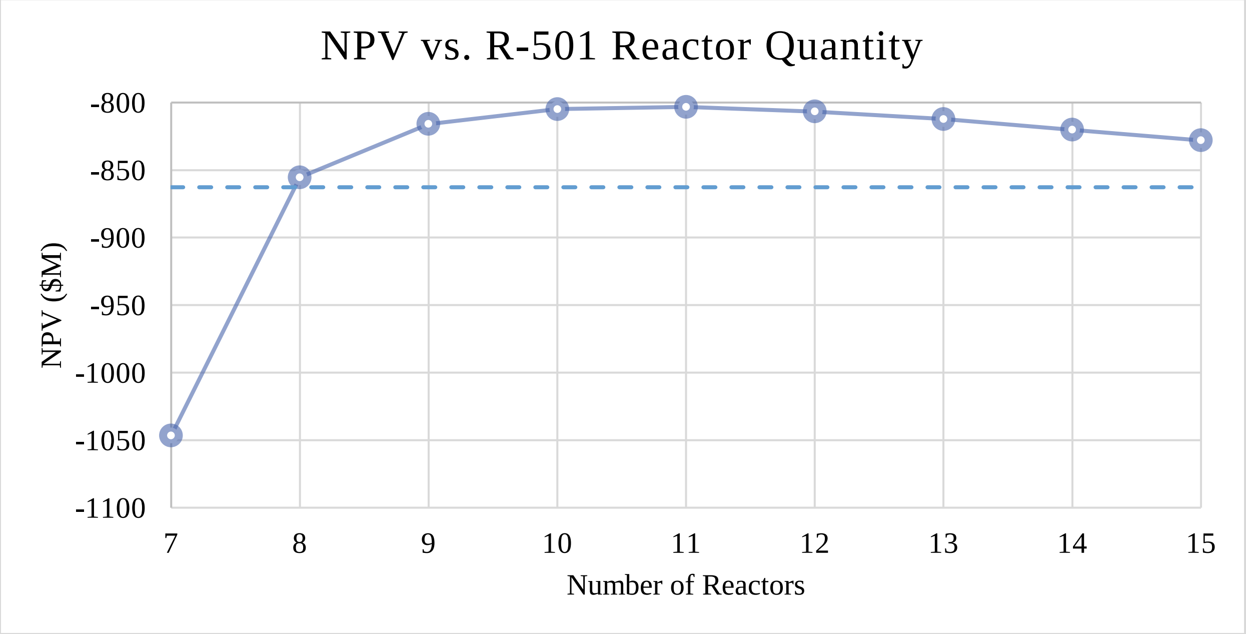

Figure 3: *NPV vs. R-501 Reactor Quantity.*

This optimization may be noted from Figure 3; keep in mind that the solid line denotes optimization curve and dashed line denotes base case NPV. Compared to the base case NPV of -$863 million, removing R-502 a-e and utilizing 11 reactors in R-501 resulted in an NPV of -$803 million. Since the NPV increased by $59 million compared to the base case, the removal of R-502 a-e and E-502 was implemented. The new series of parallel reactors was named R-501 a-k to represent the 11 reactors.

The next variable optimized was the length to diameter (or L/D) ratio of each reactor in R-501 a-k. This value was manipulated by varying reactor length with diameter held constant. Heuristics limit the value for L/D to be between 2-10.

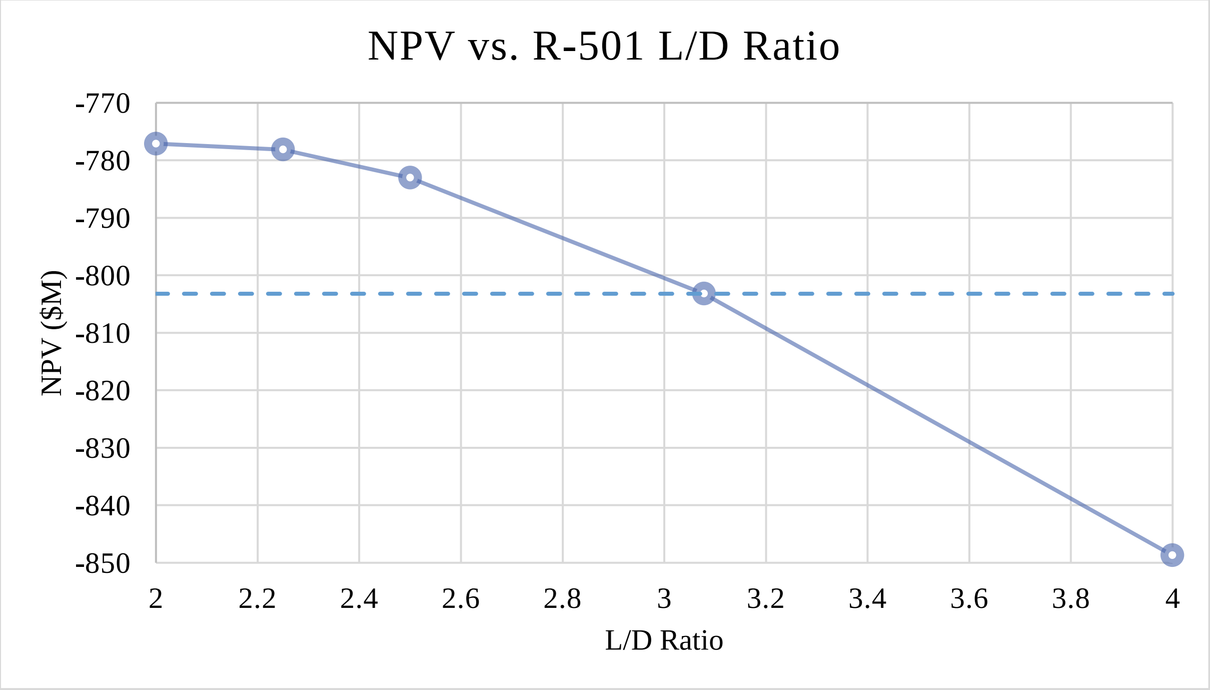

Figure 4: *Reactor Quantity vs. L/D Ratio.*

A clear optimum L/D ratio was determined to be 2 as seen in Figure 4. From here out, the solid line denotes optimization curve and dashed line denotes previous case NPV. The reactor length associated with this ratio is 6.4 meters. At this L/D ratio, the NPV was calculated to be -$777 million. One consideration to note with the process of optimizing the L/D ratio is that since diameter was held constant and length was varied, both the L/D ratio and reactor volume were changing. This curve does not accurately reflect the direct impact of changing L/D ratio on the NPV since volume was changing as well. Therefore, for future optimizations, it is recommended to vary L/D with volume held constant and to vary volume with L/D held constant to more accurately demonstrate the impact of these changes on NPV.

The next variable optimized was reactor inlet pressure, in which the optimization can be viewed in Figure 5:

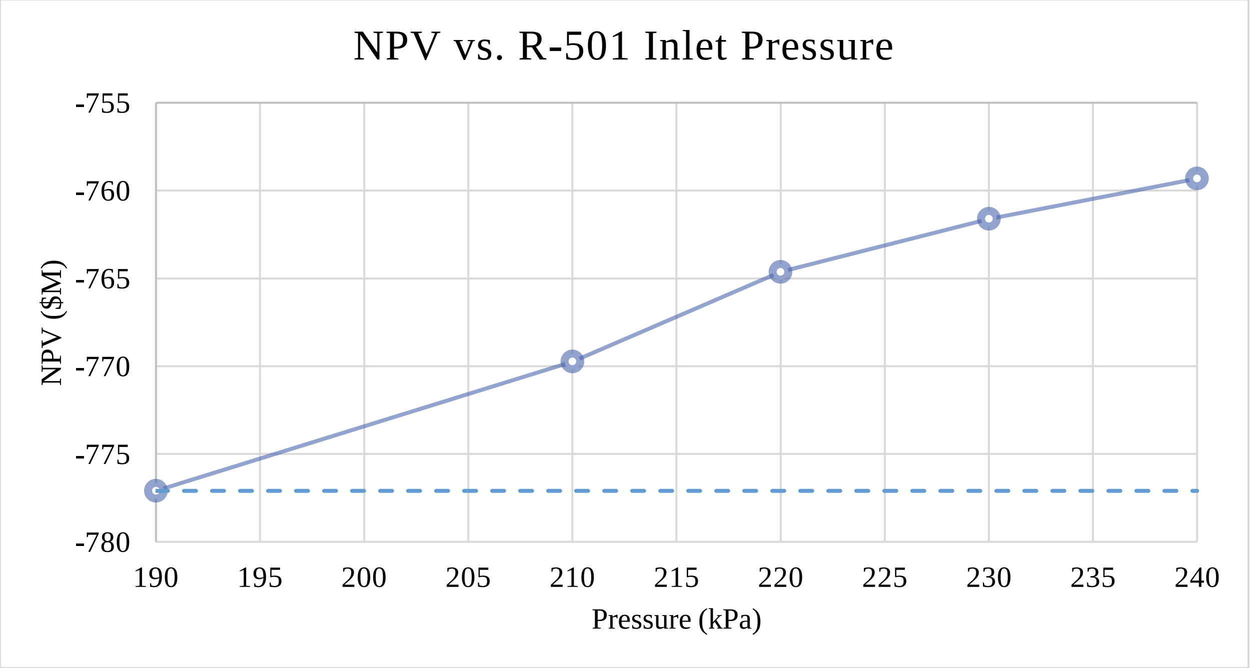

Figure 5: *NPV vs. R-501 Inlet Pressure.*

A clear trend of increasing NPV with increasing inlet pressure was seen in Figure 5. Note that the solid line denotes optimization curve and dashed line denotes previous case NPV. Per Turton$_1$, the highest design pressure for the reactor was 264 kilopascals. To avoid operating at the maximum pressure, a safety factor of 10% was implemented, and 240 kPa was determined to be the maximum pressure to be used during optimization. This safety factor accounts for potential fluctuations in pressure during operations. The NPV associated with an inlet pressure of 240 kPa was -$759 million.

The final variable manipulated for R-501 was the reactor inlet temperature. Within the PRO/II simulation, the reactor inlet temperature was primarily controlled by the flowrate of high-pressure steam in stream 4. Within the base case PRO/II file, a controller was used to vary the flowrate of stream 4 to set the temperature of the reactor feed to a certain value. During the optimization of the reactor feed temperature, the controller was disabled, and the flowrate of steam was varied manually.

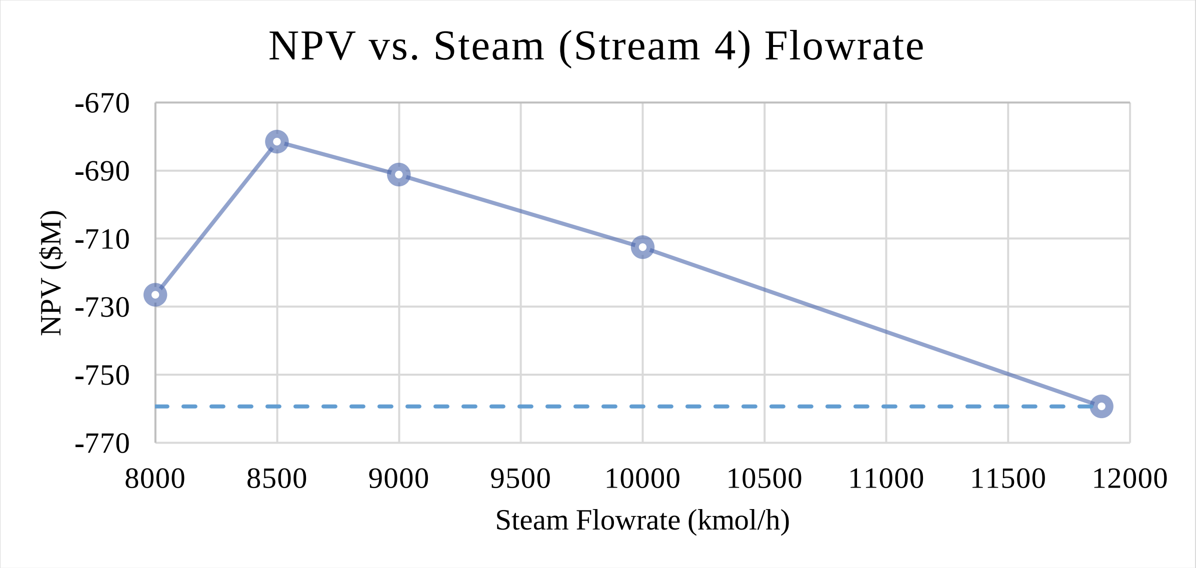

Figure 6: *NPV vs. Stream 4 Flowrate.*

An optimum flowrate of high-pressure steam was found to be 8500 kilomoles per hour, which corresponded to a reactor feed temperature of 560^{o}C and an NPV of -$681 million. Note from Figure 6 that the solid line denotes optimization curve and dashed line denotes previous case NPV. Once this optimum was established, the controller was re-enabled, and set to change the flowrate of stream 4 to maintain the temperature of 560^{o}C. An item to note for the process followed of optimizing the steam flowrate is that two variables were changing as steam flowrate was changing: concentration of reactants in R-501 and R-501 feed temperature. For future optimizations, it is recommended to optimize steam flowrate with R-501 feed temperature held constant and to optimize R-501 feed temperature with steam flowrate held constant to achieve a better optimization which more accurately reflects the impact of the individual variables on the NPV. Completion of the optimization of R-501 resulted in an overall increase in NPV of $181 million.

The next variable considered was the operating pressure of the three-phase separator (V-501). The optimum operating pressure for V-501 did not deviate from the base case value of 185 kPa, so no changes in NPV were observed following the optimization of the three-phase separator's operating pressure. Pressure was manipulated by varying the outlet pressure within E-505. First, the changes were simply evaluated. Had a decrease in pressure resulted in an increase in NPV, a valve would have been added. Likewise, if an increase in pressure resulted in an increase in NPV, a pump would have been added and priced. However, since both changes resulted in a lower NPV, neither piece of equipment was necessary.

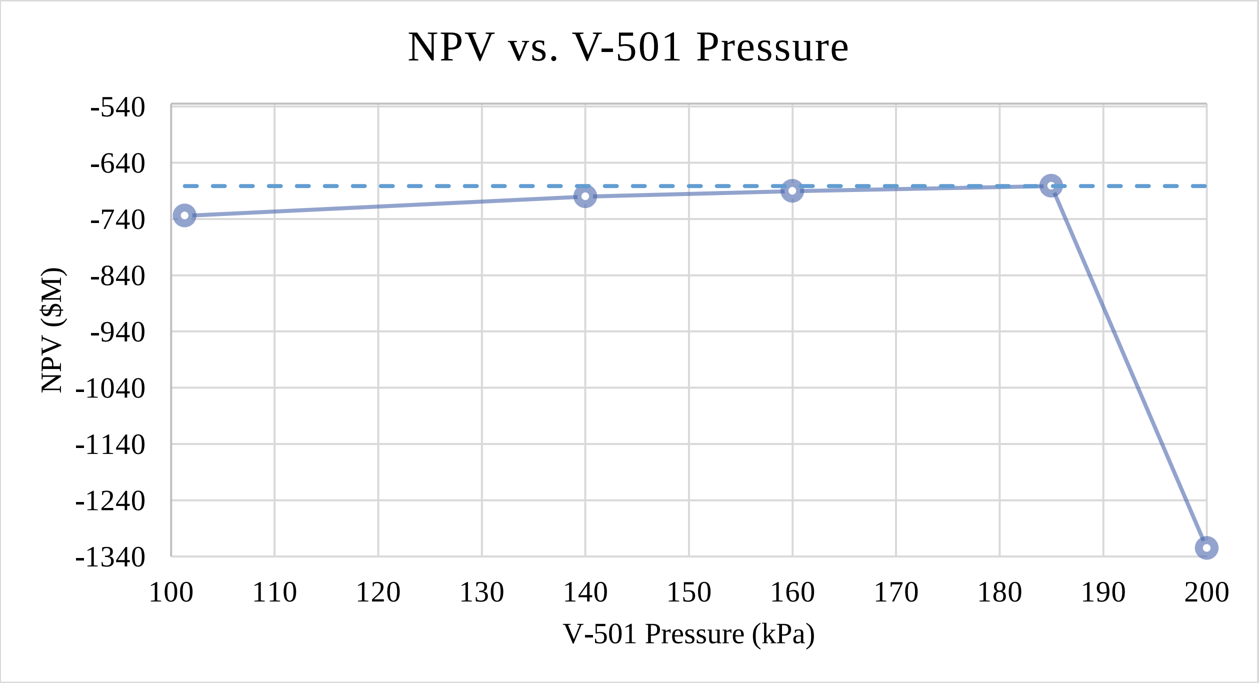

Figure 7: *NPV vs. V-501 Feed Pressure.*

Note from Figure 7 that the solid line denotes optimization curve and dashed line denotes previous case NPV. The significant decrease in NPV which occurred when pressure increased was due to the change of the partition coefficients for the mixture. Increasing pressure caused a change in the partition coefficients such that more vapor entered the organic phase. This resulted in a decreased flowrate of the benzene/toluene product stream and more difficult separations.

The second variable to consider for the three-phase separator was the feed temperature. This value was controlled by the heat exchanger network prior to the separator. Specifically, the outlet temperature of E-505 dictated the feed temperature to the three-phase separator. Optimization of the feed temperature for the three-phase separator, V-501, was achieved by varying the outlet temperature of E-505.

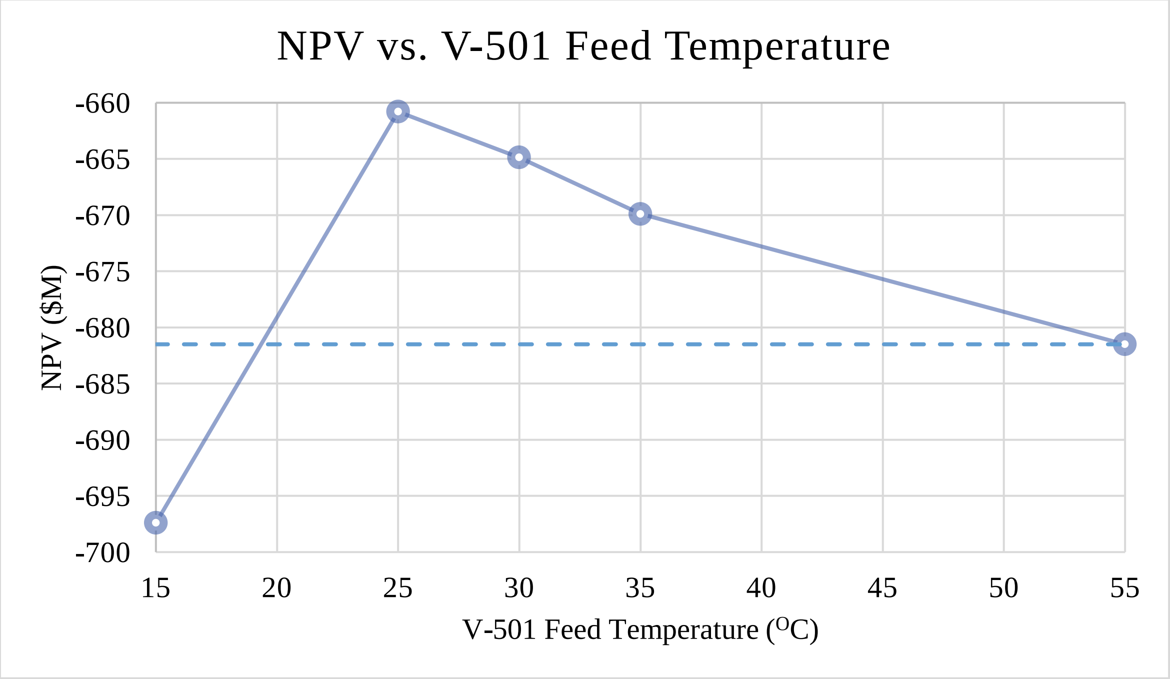

Figure 8: *NPV vs. V-501 Feed Temperature.*

A clear trend in Figure 8 displayed that increasing NPV with decreasing feed temperature was observed during the optimization of the feed temperature for V-501 until 15^{o}C was reached. The Solid line denotes optimization curve and dashed line denotes previous case NPV. The utility in E-505 was switched from cooling water to refrigerated water in order to allow for a further decrease in feed temperature. The points at 25, 30, and 35^{o}C used a refrigerated water utility. The feed temperature using refrigerated water was limited to 25^{o}C at its lowest due to this being the minimum approach temperature for refrigerated water. Further decreasing the feed temperature for V-501 required a colder utility. The use of a refrigerant was considered for the point at 15^{o}C, but due to the significant increase in utility cost, it was decided that refrigerated water would be the better option. Changing the feed temperature resulted in an NPV increase of $21 million compared to the previous case.

Next, the separations section of the process was optimized. No significant changes in distillation column operating temperature or pressure were found because the number of trays within the towers were continuously updated (hence, the shortcut columns were also updated) to meet the process requirements. Thus, the tower construction was being updated to match the process operating conditions. It was found that changes in certain recoveries for the towers caused significant impacts on the NPV.

Prior to conducting tower optimizations, it was immediately noticed that the material of construction for T-501 and T-502 was titanium in the base case. From previous knowledge, the team knew that stainless steel would be a sufficient material of construction. The material of construction was changed to stainless steel for T-501 and T-502, resulting in an NPV increase of $95 million.

The assumption was made that the purity of the distillate for T-501 could not be altered, since the fuel gas and benzene/toluene products were being sold. However, the toluene recovery to the distillate for T-501 was optimized as this value did not affect the quality of product being sold. The results of this optimization are seen in Figure 9; For the following two figures, the solid line denotes optimization curve and dashed line denotes previous case NPV.

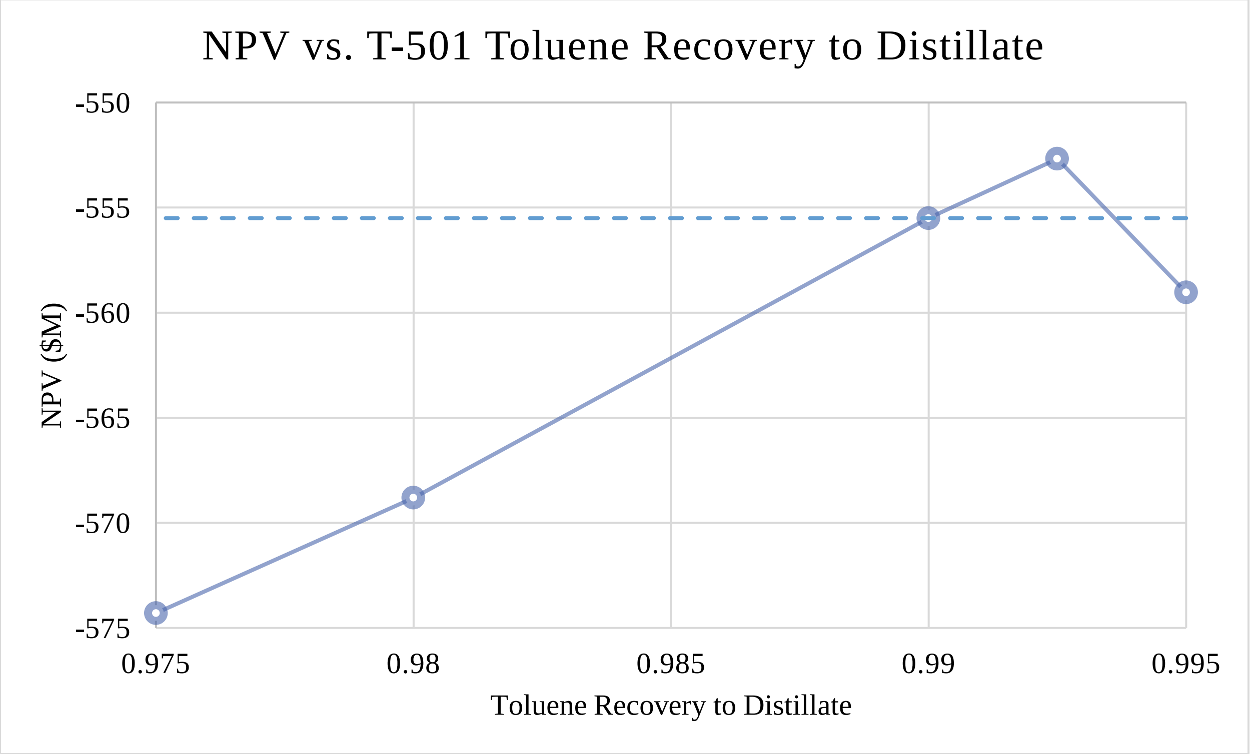

Figure 9: *NPV vs. T-501 Toluene Recovery to the Distillate.*

An optimum recovery of toluene to the distillate was found to be 0.9925 (or 99.25%) which corresponded to an NPV of -$553 million. A similar process was followed for the optimization of T-502. Knowing that the purity of the styrene product leaving the bottoms of T-502 could not be altered, the column’s overall styrene recovery was optimized. Changing this value changed the amount of styrene present in the recycle and the number of trays needed in T-502.

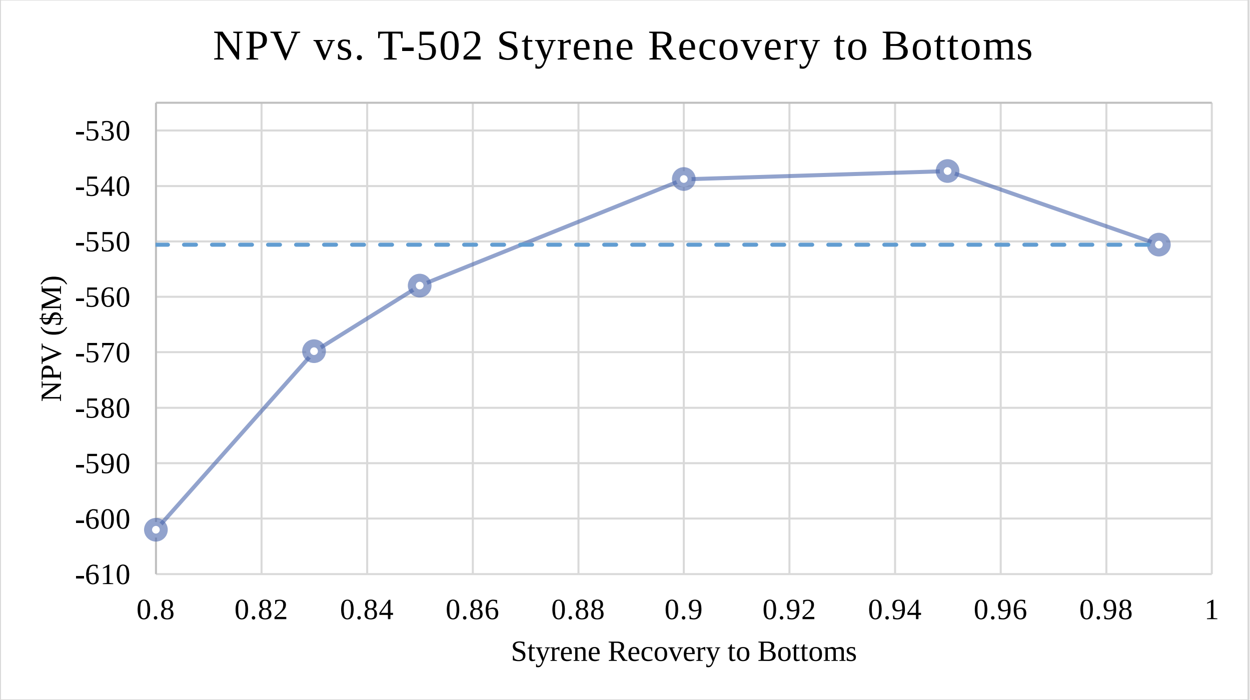

Figure 10: *NPV vs. T-501 Toluene Recovery to the Distillate.*

As seen in Figure 10 above, an optimum styrene recovery to the bottoms was found to be 0.95 (or 95%) compared to the original value of 0.99. The NPV associated with this optimization was -$537 million.

Following more thorough review of the PRO/II and economic model, a few changes were required at this point. Per Turton$_1$, the maximum outlet to inlet pressure ratio for a compressor is 3. The initial value of this ratio for C-501 was 6, so a second compressor, C-502, was added as required. An intercooler was also added between the two compressors to ensure that the outlet temperature from C-502 met process specifications. Additionally, the assumption was made that throughout optimization, updates to zone analysis would result in minimal changes to the NPV. Zone analysis was performed for the final optimized model, and C-502 was added. The NPV resulting from these changes was -$568 million. After further review of the distillation column material of construction, it was decided that carbon steel would be an appropriate material of construction for the towers due to their operating conditions and the components present within the towers. Changing the material of construction further increased the NPV to a value of -$525 million. The management team recommended the addition of an intermediate heat exchanger, E-510, between C-501 and C-502. Inclusion of this increased NPV by less than $1 million, so the final rounded NPV remained the same at -$525 million.

The table below summarizes the final metrics for the optimized styrene production process:

Table 2: *Summary of Optimized Case Metrics*

Net Present Value ($M)	Annual Equivalent ($M)	Fixed Capital Investment ($M)
-525	-85	-90

As demonstrated by the table above, the cost of making styrene in-house would be $525 million more than the cost of purchasing the styrene. This value corresponds to a break-even price of $2,015 per tonne of styrene whereas the purchase price of styrene is $1,598 per tonne. The difference in these prices is $417 per tonne of styrene which should be viewed as the risk reduction premium of making styrene in-house.

A MUMNE (minimum utility, minimum exchangers) analysis was performed for heat exchangers E-501 through E-505. It was found that as an alternative to the use of HPS to heat stream 2, the reactor effluent (stream 10) could be used for this. E-503 was reconfigured to exclude high pressure steam in favor of exchanging heat between streams 2 and 10. Additionally, E-501 was re-configured in a similar way to exchange heat between streams 2 and 14. E-504 and E-505 were considered for possible heat transfer substitution, but attempting to utilize either exchanger would result either in temperature crossover or inadequate heat transfer for process streams prior to V-501. The substitution of reactor effluent as the hot side stream for E-501 does save on the cost of utilities, however during start up, a utility needs to be used to heat E-501 until the process reaches steady state, as the flow in E-503 will be insufficient to heat the fresh feed until it reaches steady state.

The exchangers within the distillation columns, E-506 through E-509, were not considered for optimization as their requirements were dependent on process specifications, and changing their parameters may result in issues within the distillation towers.

The table below summarizes the operations of the modified heat exchangers considering MUMNE analysis. This table should be used in conjunction with the *Optimized PFD with MUMNE* provided on the following page.

Table 3: *MUMNE Affected Streams List*

	E-501	E-503
Cold Side In	2b	2a
Hot Side In	14	10
Cold Side Out	3	2b
Hot Side Out	14b	13

Performing MUMNE resulted in an NPV increase of only $3 million. Taking into consideration the substantial difficulties of implementing these changes during start-up, it is not recommended to pursue this option, and, therefore, the increase in NPV will not be considered in the project metrics discussed.

MUMNE PROCESS FLOW DIAGRAM

Styrene from Ethylbenzene: Optimized Process Flow Diagram with MUMNE

Heat Exchangers	
E-501 Feed Heater	E-506 Reboiler
E-503 Product Cooler	E-507 Condenser
E-504 Product Cooler	E-508 Reboiler
E-505 Product Cooler	E-509 Condenser

Pumps & Compressors	
P-501 A/B Wastewater Pump	P-506 A/B Recycle Pump
P-502 A/B Reflux Pump	C-501 Fuel Gas Compressor
P-503 A/B Reflux Pump	C-502 Fuel Gas Compressor
P-504 A/B Benzene/Toluene Pump	
P-505 A/B Styrene Pump	

Vessels	
V-501 3-Phase Separator	V-503 Reflux Drum
V-502 Reflux Drum	

Towers	
T-501 Benzene/Toluene Column	T-502 Styrene Column

Reactors
R-501a-k Ethylbenzene to Styrene Reactors

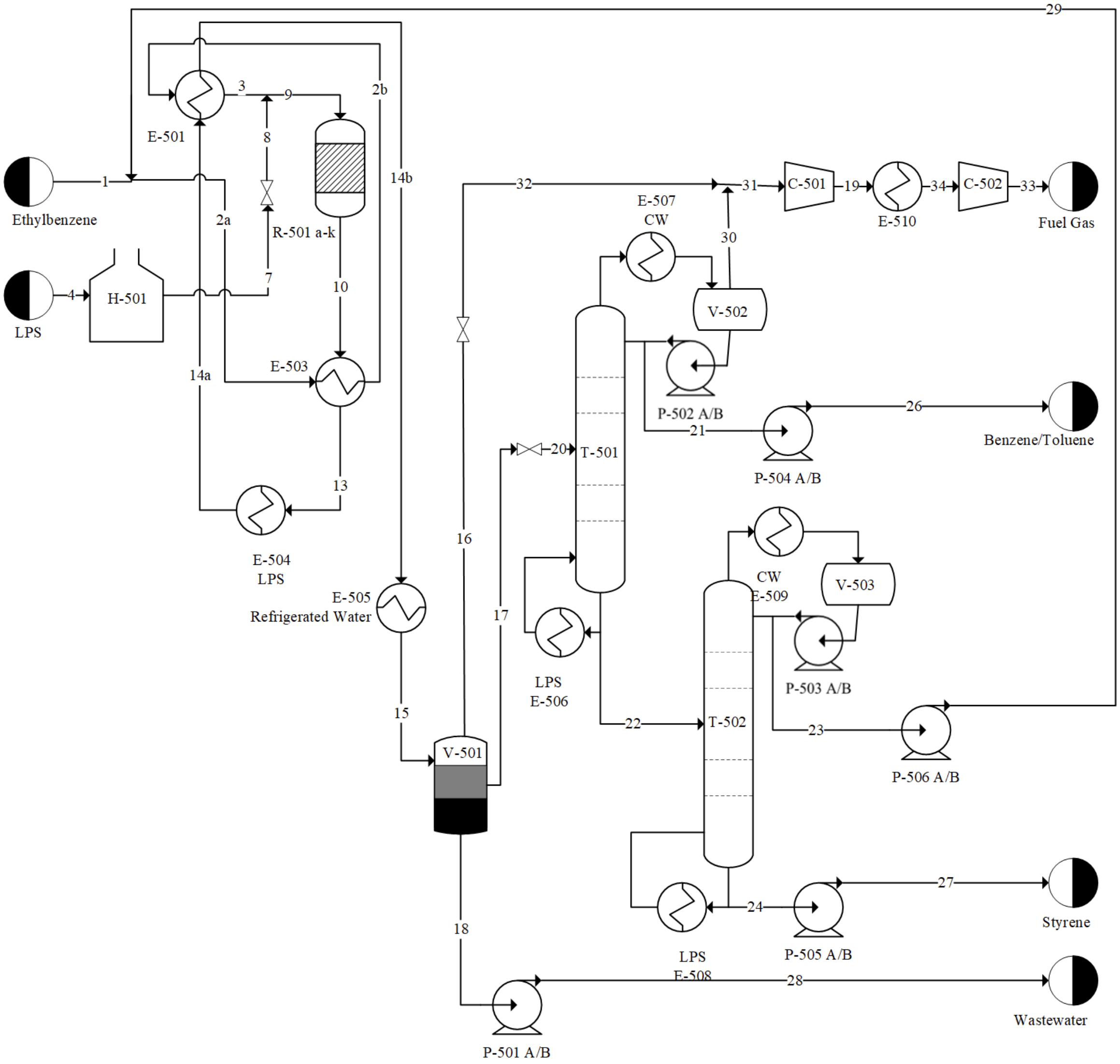

Figure 11: *MUMNE Optimized Process Flow Diagram*

ADDITIONAL OPTIMIZATION: ISOTHERMAL REACTOR

In addition to the optimizations towards the styrene production facility above, I was tasked with optimizing a separate isothermal styrene reactor. While this individual reactor utilizes the same reaction mechanisms as in Unit 500, it utilizes a fluidized bed rather than an adiabatic reactor; while fluidized beds have more complex design and are more prone to catalyst erosion, they offer greater heat transfer capabilities and particle size compatibility than the adiabatic reactor used for Unit 500[2]. This reactor had predefined feed and conditions, which may be seen in Table 4 below; some of these conditions were further defined by the parameters within Coco et al[2]:

***Table 4:** Constraints for Isothermal Styrene Reactor Optimization*

Condition	**Parameters**
Feed Conditions:	8000 kmol/hr H_2O 512.7 kmol/hr Ethyl Benzene 1.2 kmol/hr Styrene 1.8 kmol/hr Benzene 2.13 kmol/hr Toluene
Pressure Range:	From .75 to 5 barg
Temperature Range:	From 300^o to 750^o C
Tube Length Range	From 6.1 to 10 meters
Length/Diameter Range:	From 2 to 10
Additional Information	Particle Diameter = 1 millimeter Void Fraction = .45 10% of feed into the reactor bypasses without reaction Must operate at 3-10 times minimum fluidizing velocity

Unlike the optimizations around Unit 500, this separate reactor was tasked to be optimized around the selectivity of styrene, with a minimum required single pass conversion of 5%. The reactor was modeled into AVEVA PRO/II simulation software. The simulation was designed so that the parameters seen in Table 4 are used as base stream data, and a set of controllers, calculators and an optimizer were used to determine the maximum selectivity conditions for the fluidized bed. The final simulated model of the reactor can be seen in Figure 12 below:

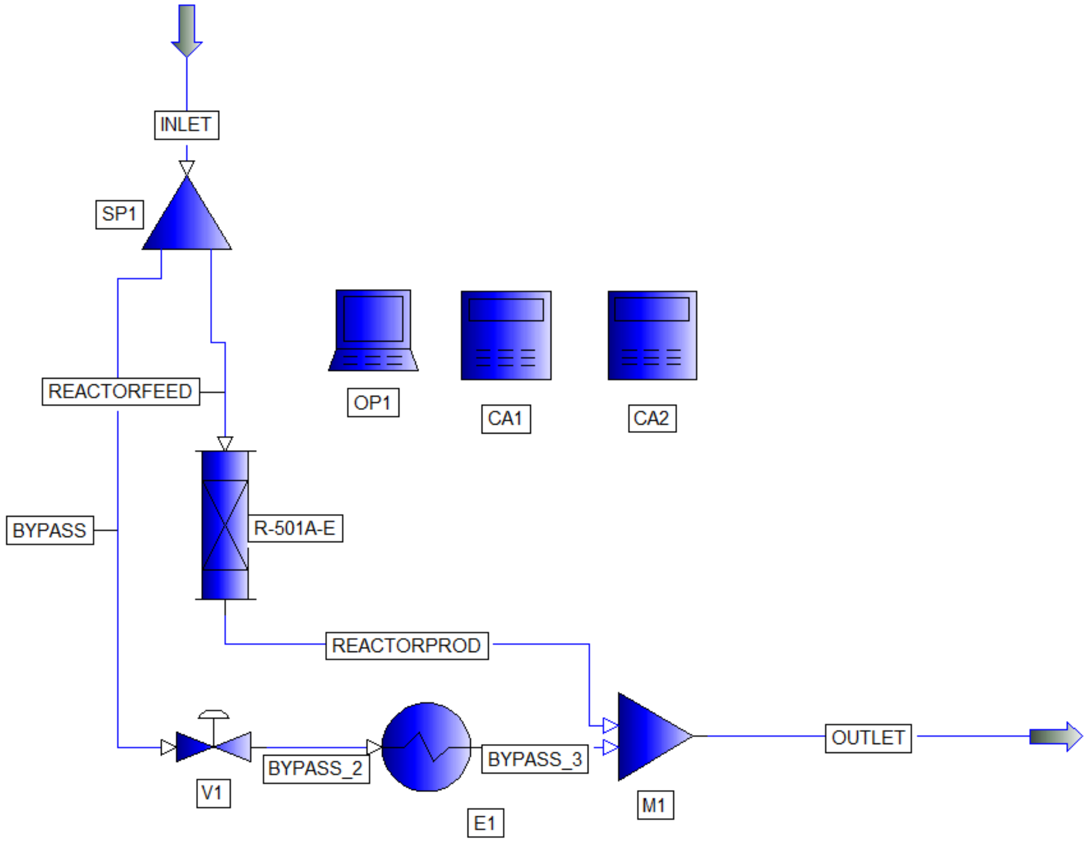

Figure 12: *Simulated PRO/II Isothermal Styrene Reactor*

The bypass streams alongside the reactor were added to represent the 10% bypass of feed through the reactor as per the design prompt provided in Table 4, with both a valve and exchanger added along the bypass to simulate the same pressure and temperature drop the reactor uses. The first calculator, labeled “CA1” was used to find the values for process parameters that will be checked by the optimizer “OP1”, as well as finding the selectivity to styrene for the reactor. The second calculator, “CA2” was used to confirm that the velocity through the reactor was within the required fluidizing velocity range cited in Table 4 that is typically recommended for fluidized bed operation$_2$.

The optimum conditions were determined through the OP1. First, an optimum temperature was found to be 493^{o}C; increasing temperature past this point increased the likelihood of side reactions occurring over the styrene reaction, resulting in a decrease in the styrene selectivity objective function, and decreasing temperature reduced overall conversion and therefore styrene product. Next, the optimum pressure was 3.97 bar gauge, which is on the higher end of the range due to the correlation between partial pressure and concentrations both trending directly with reaction rate. Lower pressures mean lower overall conversion, while higher pressures past this point favor side reactions, much like the trend noticed for temperature. The reactor volume optimum was found to favor minimum length-to-diameter ratio and maximum tube length, indicating that the reactor volume favors the largest possible tube length and largest tube diameter within the length-to-diameter design parameters, and therefore the largest reactor volume possible at 50 m^3. Maximized reactor volume increases the overall conversion in addition to increasing the pressure drop, which correlates to more interaction of reactants with the catalyst and therefore higher overall conversion and therefore higher selectivity to styrene.

CONCLUSIONS AND RECOMMENDATIONS

After completion of optimization of the styrene production plant the final NPV was -$525 million. This value is the additional cost of making styrene compared to purchasing styrene. When comparing the economics of making styrene and buying styrene, this is equivalent to a risk premium of $417 per tonne of styrene. It is recommended to conduct a secondary optimization cycle in order to address additional areas for improvement in the process. First, it is recommended to optimize the volume of each individual reactor with the L/D ratio held constant after the optimum number of reactors is found. Once the optimum volume is found, the L/D ratio should be optimized with volume held constant. Finally, to optimize the temperature into the reactor the temperature of the steam leaving of the fired heater should be optimized with the flowrate held constant. Once that optimum is found, the flowrate of steam should be varied with the reactor feed temperature held constant in order to find the optimum steam flowrate.

There are some hazards that should be considered in this process. The two towers as well as their respective reflux drums operate at vacuum, which requires special design to ensure safety. There are some dangers of operating at a vacuum which includes the implosion of a failed vacuum vessel. It is important to have pressure relief valves and adequate safety factors on components of the tower. Since there are flammable components in this process, all pressure relief valves should vent to a safe location. This low pressure is necessary to help prevent spontaneous polymerization of styrene. There is a risk of spontaneous polymerization at temperatures above 125^oC, so temperature sensors and control loops should be present to minimize spontaneous polymerization risk. It is also recommended that current operating conditions of T-502 are maintained in the process to minimize this risk. There are potential environmental and health concerns with excessive exposure to some of the components in this process which will require the company to strictly adhere to EPA and OSHA guidelines.

It is recommended to conduct a thorough and detailed market study on the reliability and availability of styrene. This market study can be used to determine if building the styrene production plant is favored over purchasing styrene. A preliminary market study was completed and it was determined that although the price of styrene is currently consistent, there is minimal styrene sold on the open market. This suggests that styrene production is most often used to make a different product of higher value, such as polystyrene. When considering this option, it is recommended to continue with the construction of the styrene plant as the profit of polystyrene will likely offset the losses in the styrene plant.

APPENDICES

The following files have been attached with the submission of this report:

1. Appendix 1: Base case PRO/II simulation – “ChE 450 – Thesis Report – Appendix 1”
2. Appendix 2: Base case economic model – “ChE 450 – Thesis Report – Appendix 2”
3. Appendix 3: Optimized PRO/II simulation – “ChE 450 – Thesis Report – Appendix 3”
4. Appendix 4: Optimized economic model – “ChE 450 – Thesis Report – Appendix 4”
5. Appendix 5: Optimized isothermal reactor PRO/II simulation – “ChE 450 – Thesis Report – Appendix 5”

REFERENCES

1: Turton et al.(2018). *Analysis, Synthesis and Design of Chemical Processes.* Pearson Publishing.

2: Coco et al (2014). *Introduction to Fluidization.* American Institute of Chemical Engineers.