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## Optimization of a Styrene Production and Separation Process

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OPTIMIZATION OF A STYRENE PRODUCTION AND SEPARATION PROCESS

By  
Bryce Little

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

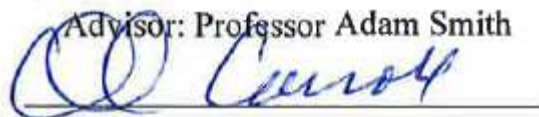
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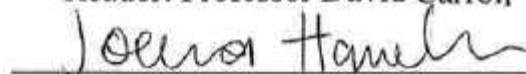
Approved By

A handwritten signature in black ink, appearing to be 'A. Smith', written over a horizontal line.

Advisor: Professor Adam Smith

A handwritten signature in blue ink, appearing to be 'D. Carroll', written over a horizontal line.

Reader: Professor David Carroll

A handwritten signature in black ink, appearing to be 'Joanna Harrelson', written over a horizontal line.

Reader: Professor Joanna Harrelson

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## ABSTRACT

Bryce Little: OPTIMIZATION OF A STYRENE PRODUCTION AND SEPARATION  
PROCESS (Under the direction of Dr. Adam Smith)

A step wise optimization of Unit 500 was completed. Unit 500 is a planned ethylbenzene to styrene production plant that has a annual production goal of 100,000 metric tons of styrene. The cost of styrene on the market is \$1,598. The base case of Unit 500 produced styrene at a cost of \$2,650. Optimization was completed with an emphasis on parametric changes though material of construction and heat integration were also considered. The optimized Unit 500 design reduced the cost of styrene production to \$2,035 per metric ton. While this represents a significant improvement on the base case cost, it is not competitive with the market cost of styrene. At this stage, purchase of styrene at the market rate is preferable from a financial standpoint. However, risk analysis is required to better understand the implications of market purchase. Additionally, further optimizations should be pursued on Unit 500 while alternatives to the process currently described in Unit 500 for the production of styrene.

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## **Project Introduction**

Unit 500 is a proposed production unit that makes styrene, the monomer of polystyrene. This unit produces styrene by the dehydrogenation of ethylbenzene. A base case for this unit was created to achieve a production rate of 100,000 metric tons per year. This base case was highly unattractive from a financial perspective compared to the purchase of styrene. The Base Case NPV of Unit 500 was approximately \$(919) million. The cost to produce styrene was \$2,650 per metric ton. Styrene has a market price of \$1,598 per metric ton. Though producing styrene was more expensive than the purchasing, Unit 500 provided some key benefits such as control of styrene supply that was not limited to styrene availability and qualities on the market. Unit 500 provided a greater level of control over the quality and quantity of styrene to produced. As such, further analysis was completed on the base case in an attempt to improve the NPV of Unit 500.

A stepwise optimization was completed in order to increase the financial attractiveness of Unit 500. The optimization of this process focused primarily on parametric variables in Unit 500. However, material of construction and heat integration were also considered during the optimization of the process. The goal of this optimization was to reduce the styrene manufacture price per metric ton. The NPV was improved to \$(534) million for an NPV savings of \$385 million. This corresponded to a styrene production cost of \$2,035 per metric ton. This is still higher than the market price of styrene and Unit 500 remains unattractive from a financial perspective. A risk analysis should be performed in order to quantify the risk associated with market stability and ability to meet demand at required styrene quality. If the risk associated with

the market is greater, there may still be merit to the construction of Unit 500 in order to control production and product quality.

### **Project Description**

The goal of this project was to optimize Unit 500's Base Case NPV in order to make it a more financially attractive option compared to the alternative of the purchase of styrene on the market. Unit 500 is an ethylbenzene to styrene production plant that can produce 100,000 metric tons of styrene per year at 99.8 WT% purity. Unit 500 is designed to startup on January 1st, 2024 and operate at approximately 8,000 hours per year for a lifetime of 12 years. Unit 500 will use the reversible dehydrogenation of ethylbenzene to produce styrene. This reaction is provided below where R1 is the forward reaction and R2 is the reverse reaction.



There are also two side reactions, R3 and R4, that occur. Both consume ethylbenzene as raw materials. R3 produces benzene and ethylene. R4 produces toluene and methane. The chemical reactions are as follows:



The reactions are further described by their rate equations which provide their activation energies and can provide details to favorable conditions that maximize the particular reactions discussed above.

$$-r_1 = 6.2 \exp\left(\frac{-9,981}{RT}\right) p_{eb}$$

$$-r_2 = 6 * 10^{-5} \exp\left(\frac{-61,127}{RT}\right) p_{sty} p_{H_2}$$

$$-r_3 = 2.71 * 10^7 \exp\left(\frac{-207,989}{RT}\right) p_{eb}$$

$$-r_4 = 6.45 * 10^{-4} \exp\left(\frac{-90,981}{RT}\right) p_{eb} p_{H_2}$$

At the required 99.8 WT% styrene purity, there is risk of spontaneous polymerization at temperatures greater than 125°C. This is complicated by styrene's normal boiling point as it is higher than 125°C. As such, much of this process is run at vacuum. Spontaneous polymerization is a much lower risk at lower styrene purities.

### **Description of Base Case Process**

Fresh ethylbenzene is fed to the unit. This fresh stream meets recycled ethylbenzene from the separation section of this process. The ethylbenzene is heated, and superheated steam is then injected into the process line. This combined stream is then sent to the reactors where the dehydrogenation reactions occur. There are two banks of five packed bed reactors. Each of the five reactors are in parallel while the two banks are in series. The two banks of reactors are separated by a heat exchanger that heats the effluent of the first bank of reactors prior to being fed to the second bank of reactors. This is necessary as all of the reactions that occur are endothermic and lower the available amount of thermal energy as they progress. Following the second reactor is a set of three heat exchangers that cool and begin to condense the process stream. The partially condensed stream is fed to a three-phase separator where the different phases: liquid aqueous, liquid organic, and organic vapor are separated from one another. The liquid aqueous phase is removed as wastewater. The organic vapor stream is removed to an overhead fuel gas stream. The liquid organic stream contains majority of both styrene, the



desired product, and ethylbenzene, the raw material. It also contains toluene and benzene from the non-desired reactions. This liquid organic stream is sent to a set of two distillation columns. The first of these columns separates benzene, toluene, and any higher volatility components still within the stream from the ethylbenzene and styrene. The benzene and toluene distillate are sold as off products from this system. Some of this distillate is also sold as fuel gas. The bottoms of this first tower, primarily ethylbenzene and styrene, is sent to the second tower where ethylbenzene is separated as the distillate and recycled. The styrene bottoms stream is 99.8 WT% purity and is our final product. It is important to assure that the final product stream remains below 125°C as there is high risk of spontaneous polymerization if the stream is heated above this temperature. A PFD is provided in Appendix A.

A sensitivity analysis was performed for the base case in order to determine the sensitivity of the process to changes in various conditions. The process is most sensitive to the cost of raw material, the price of styrene, and to a lesser extent the associated equipment costs.

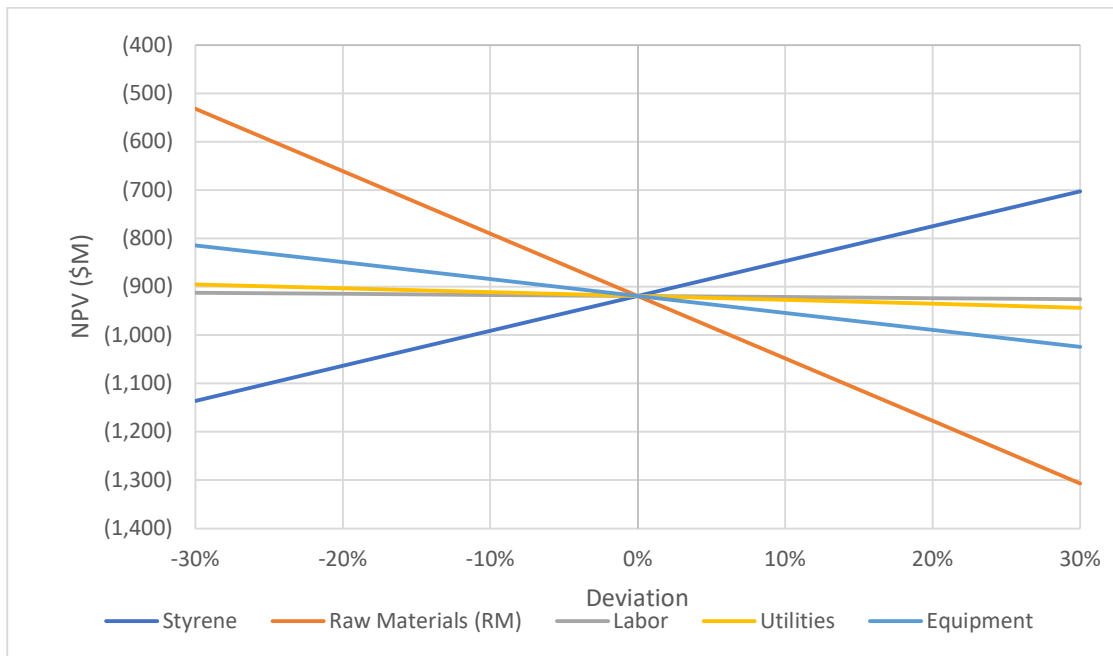


Figure 1: Sensitivity of Unit 500 Base Case

This chart indicates that raw material utilization is one of the most important considerations on the NPV of this project.

### **Description of Optimization Process**

A base case for Unit 500 was previously completed and reported upon. In this section of the project, an optimization and economic analysis was completed. The optimization was completed using “PRO/II Process Simulator” and the “Unit 500 Economic Model” Excel workbook. The optimization for this project was completed as a stepwise optimization moving from unit operation to unit operation within Unit 500. The variable being optimized was compared against values on either side of the base case value. Values were then tested until a value was found for an NPV maxima or a process constraint was reached that prevented further test values in the direction of improved NPV.

Only a single round of stepwise optimization was completed for this section of the project. While many optimizations focused on parametric changes to the unit operations, both material of construction and heat integration were also considered. NPV graphs have the tested values for each variable, the base case value is noted in red on these graphs.

### **Initial Material of Construction Optimization**

The initial material of construction for the towers was specified in the base case as titanium. It was investigated to determine if other materials of construction would be sufficient for this process. It was determined that the tower material of construction would be changed to stainless steel and NPV improved by \$74 million. Later analysis would be conducted for the use of carbon steel. This will be discussed later in “Final Tower Material of Construction Change.”

## Reactor Optimization

Reactor optimization focused on improving NPV by manipulation of the reactor that influenced equipment sizing and raw material utilization. Yield and selectivity increases allow for less raw material to be used in the production of the desired amount of styrene. Increases in the achieved conversion in the reactors allows for a reduced amount of recycle which grants savings in equipment costs. These are generally opposed within this reaction scheme and improvements in yield and selectivity are generally accompanied by losses in conversion and vice versa.

Inlet temperature to R-501 was decreased from 523°C to 516°C. This temperature was found to best balance the selectivity and conversion considerations, however, further review found that 516°C was a local maximum. This is further investigated in “Review of Selected Variables.” It should be noted that the value on the NPV charts in red is the initial process value.

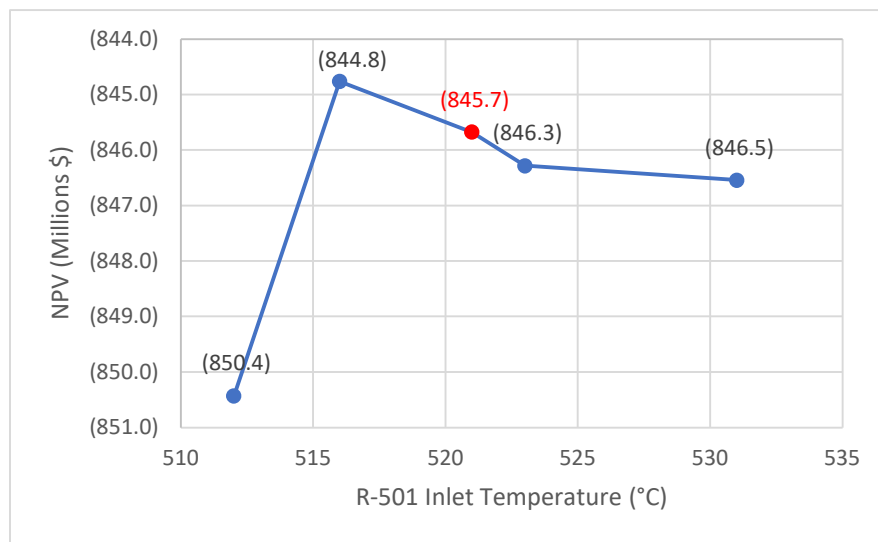


Figure 2: NPV vs R-501 Inlet Temperature

Steam was injected into the stream entering the reactors to increase the temperature and provide dilution. The added steam impacts the concentrations in the reactor influencing the reaction rate. The steam dilution was decreased from 3,900 to 3,700 kmol/hr. The steam dilution

for R-502 was not explored because the steam was added before the reactors. This variable was analyzed further in “Review of Selected Variables.”

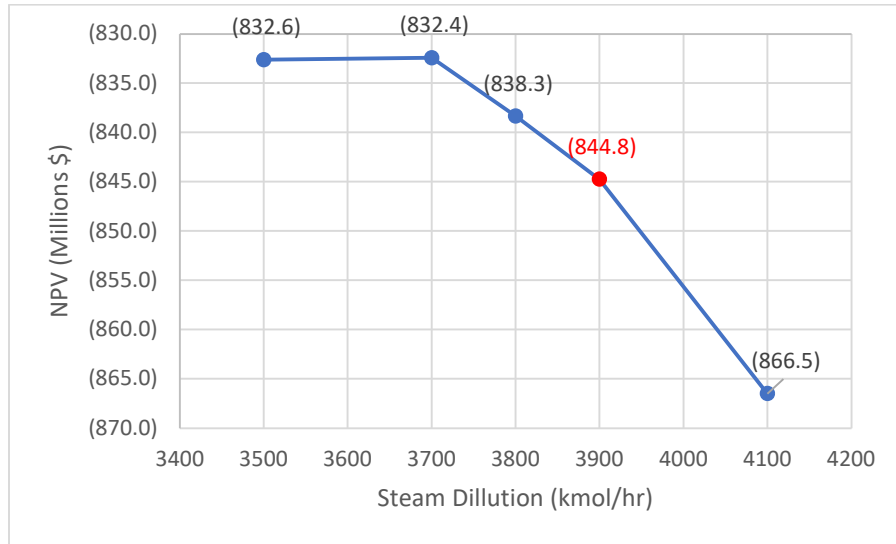


Figure 3: NPV vs Steam Dillution

Reactor R-501’s volume was decreased from 83 m<sup>3</sup> to 76 m<sup>3</sup>. R-502 was also changed at this time as it was not realized that the R-502 was defined on the basis of R-501 volume at this point.

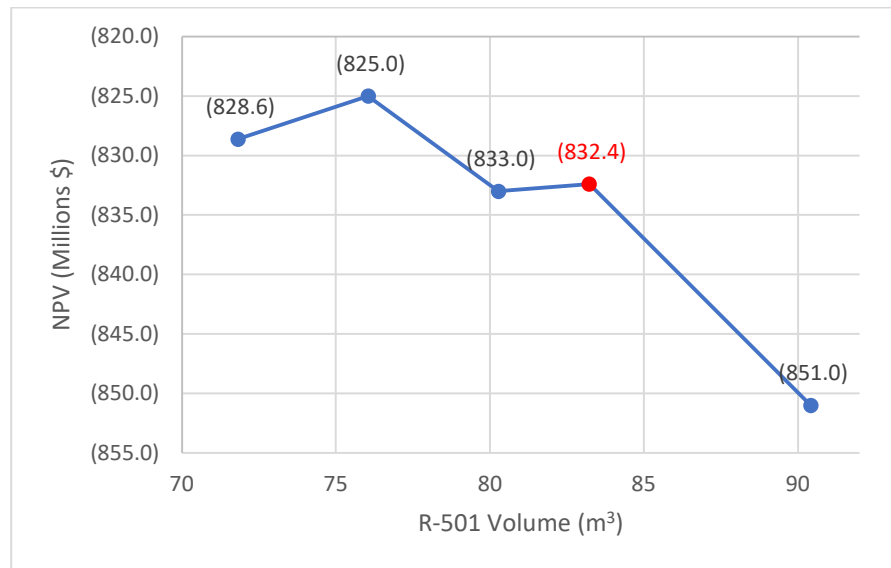
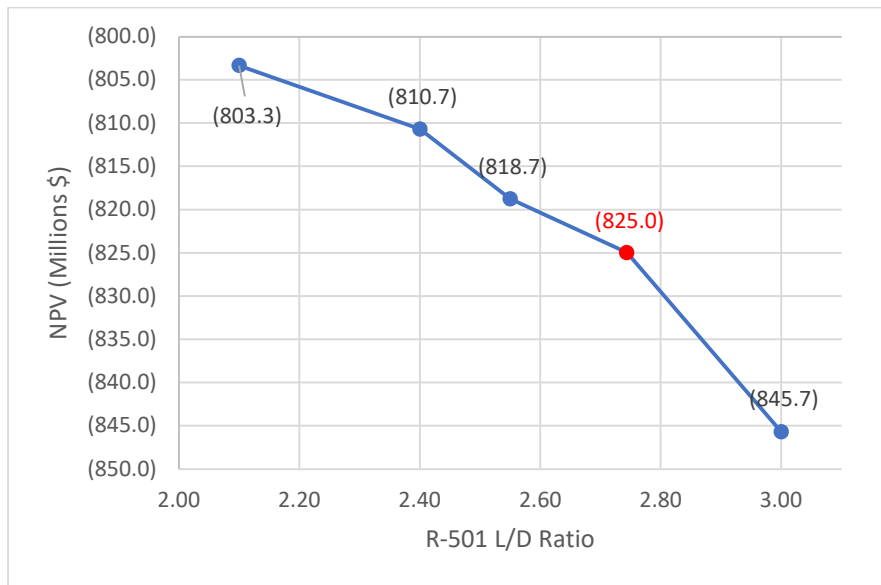


Figure 4: NPV vs R-501 Reactor Volume

The Length to Diameter (L/D) ratio impacts the pressure drop inside the reactor. The L/D ratio for R-501 was reduced from 2.74 to 2.55. The ideal ratio is closer to 2, however, due to a clerical error the 2.55 ratio was used. This error was later discovered but due to ongoing optimization a ratio of 2 was less ideal than the 2.55 ratio in use. This unfortunately likely impacted the possible amount of NPV improvement.



*Figure 5: NPV vs R-501 L/D Ratio*

Inlet pressure was then investigated. Pressure impacts the partial pressures of the components and subsequently the rates of reaction. The inlet pressure for R-501 was increased from 190 to 210 kPa.

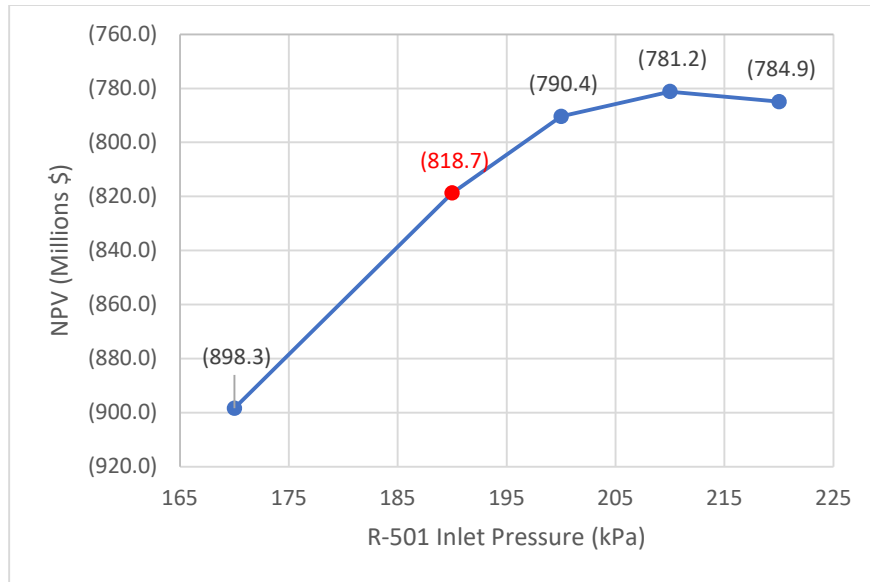


Figure 6: NPV vs R-501 Inlet Pressure

The R-502 inlet temperature was decreased from 575°C to 555°C.

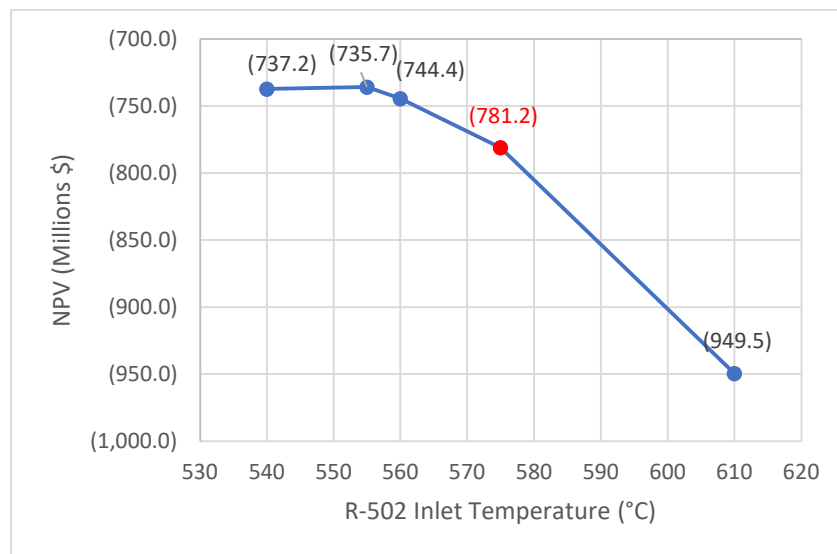


Figure 7: NPV vs R-502 Inlet Temperature

Inlet pressure in R-502 showed NPV improvement when the pressure was increased from 185 to 195 kPa for R-502. However, the cost of the compressor to increase the pressure was found to have a more negative impact on NPV than any savings from pressurization.

R-502's volume was found to be best for the NPV at the volume previously set by the R-501 reactor optimization, 76 m<sup>3</sup>.

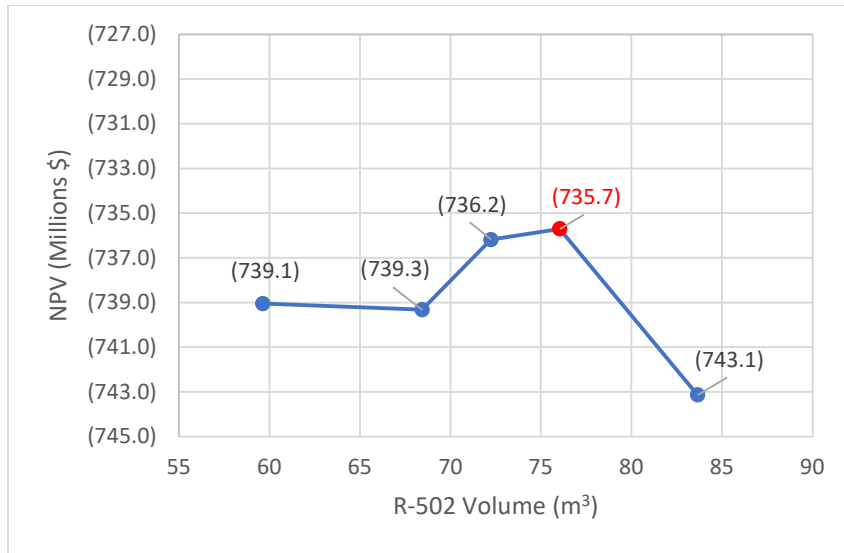


Figure 8: NPV vs R-502 Volume

As in R-501, a minimized L/D ratio was found to be best for NPV. In R-502, L/D ratio was reduced to 2 and was the lower limit on L/D ratio in this process.

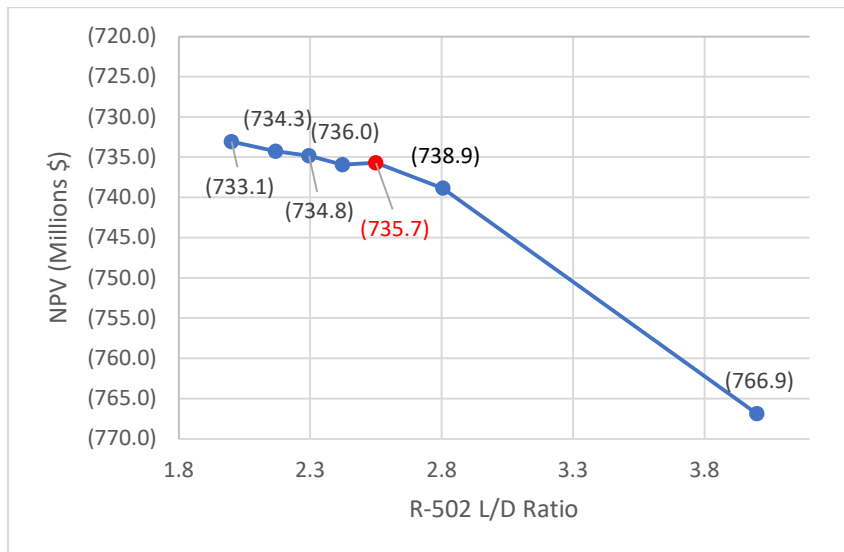


Figure 9: NPV vs R-502 L/D Ratio

### Pre-Separation Optimization

The pre-separation section cools the effluent of the reactor section. This allowed for investigation of the impact of temperature on the operation of the three-phase separator. By reducing the temperature of the pre-separation stage, less ethylbenzene and styrene was lost to

the fuel gas stream from the three-phase separator. Due to the cooling limits of cooling water (CW) preventing further optimization, refrigerated water (RW) was added to the third heat exchanger of the pre-separation. This change offset any gains from ethylbenzene and styrene recovery due to increased utility cost of RW (orange dot in figure 11). To reduce the amount of refrigerated water utility needed, an additional heat exchanger using CW was added to reduce the utility cost. RW was then used to cool the stream to 25°C. Unfortunately, the stream could have been further cooled to 10°C. This is further discussed in “Review of Selected Variables” detailed later.

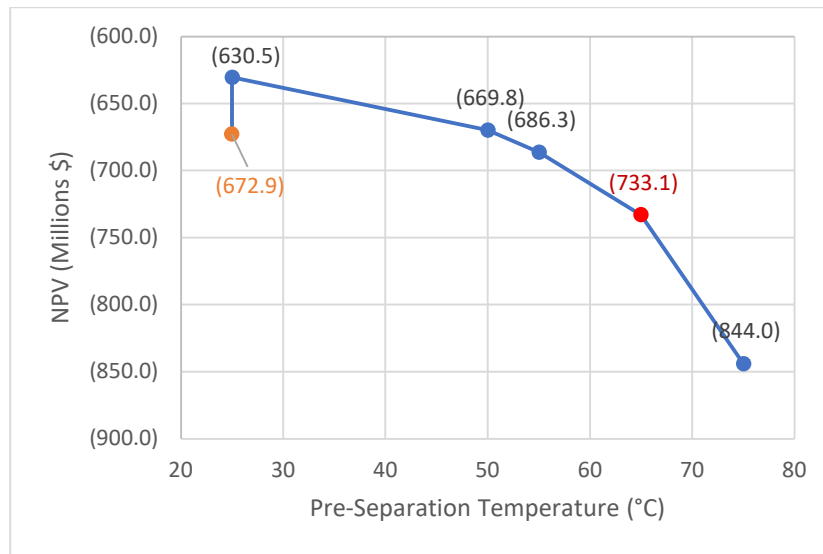


Figure 10: NPV vs Pre-Separation Temperature

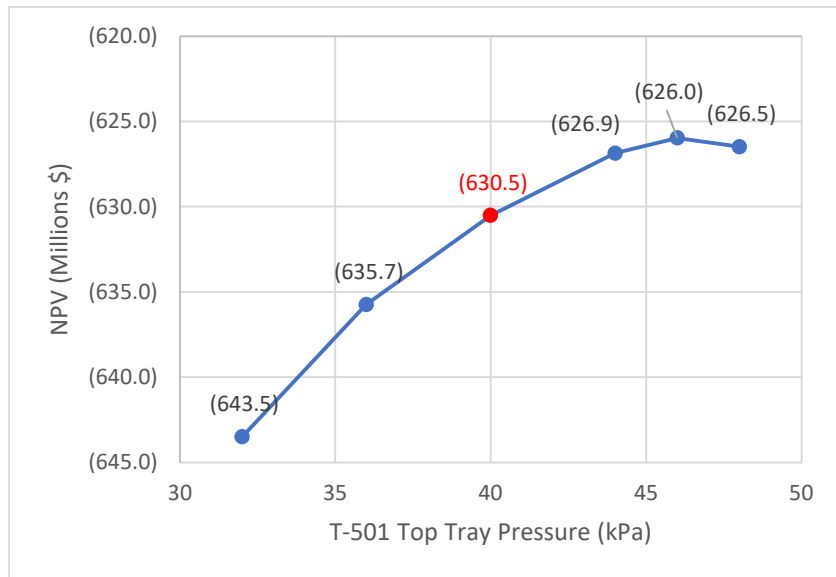
### Separation Optimization

Separation optimizations focused on the operation of the towers. The three-phase separator was not analyzed in this section as its operating temperature is controlled by the pre-separation stage of the process. The optimization of the towers included an analysis of top tray pressure, number of trays, and feed tray location for the towers. Each of these variables will have an impact on the operation of the tower. Top Tray Pressure changes the operation of the compressor and changes the reflux ratio changing the size of the column. The number of trays



changed the number of equilibrium stages within the tower. This changes the ability of the tower to achieve the separation and the required reflux ratio to achieve the desired product purity. The feed tray location refers to the tray on which the feed should enter the tower. This tray's characteristics should match the quality and composition of the feed stream.

T-501 was the first tower to be optimized. The ideal top tray pressure was found to be 46 kPa. The change in top tray pressure impacts the volume of the vapor flowing through the tower as well as the utility costs associated with condensing.



*Figure 1111: NPV vs Top Tray Pressure*

Following top tray pressure, the number of trays was optimized and the ideal number of trays was 32. Tray number changes the number of equilibrium stages. An increase in the number of stages allows for easier separations but comes incurs increased tower costs.

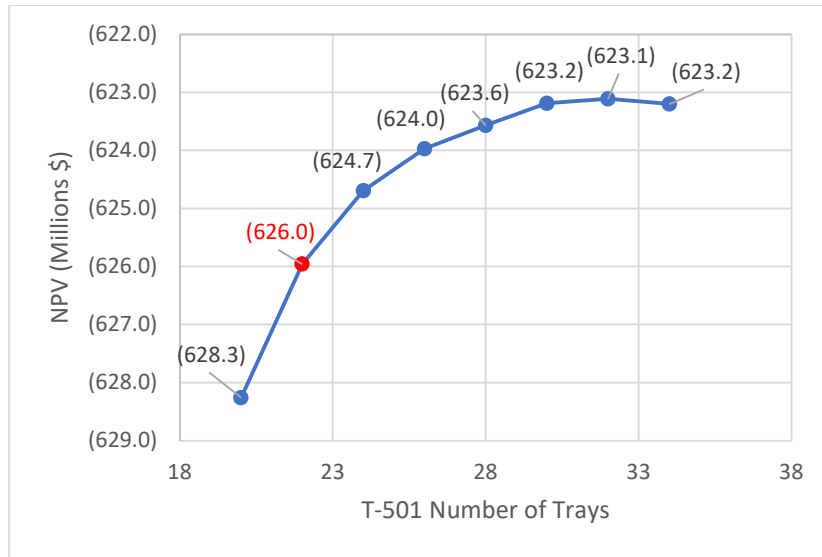


Figure 12: NPV vs T-501 Number of Trays

The feed tray location was then adjusted. The feed tray was moved from tray 8 to 9 and the change was minimal in its impact on NPV.

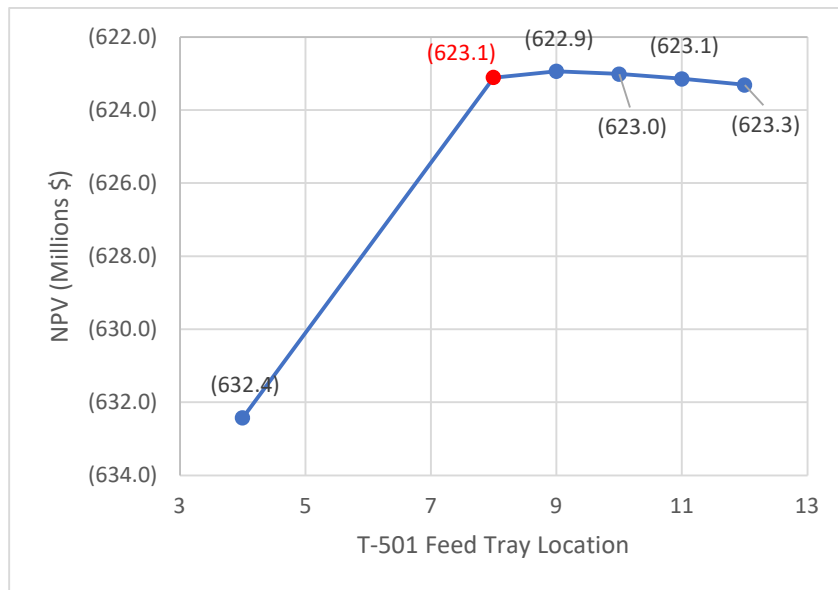


Figure 13: NPV vs T-501 Feed Tray Location

T-502 was also analyzed, though focus was on the number of trays and the feed tray location. Top tray pressure increases would increase the temperature at the bottom of the tower

increasing the risk of violating the 125°C polymerization temperature. Decreases in the top tray tower pressure were unattractive as they would increase the vapor volume in the tower and require a larger capital investment.

T-502 number of trays decreased from the base case value of 70 to 66 trays.

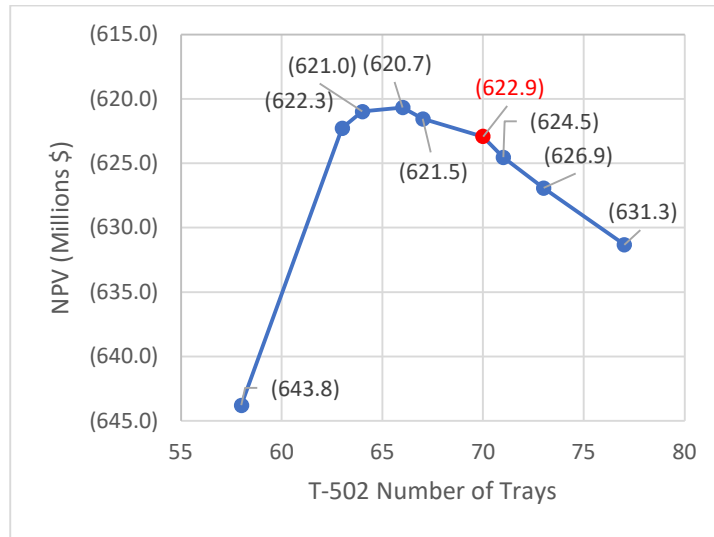


Figure 14: NPV vs T-502 Number of Trays

The feed tray location was moved from tray 25 to tray 31.

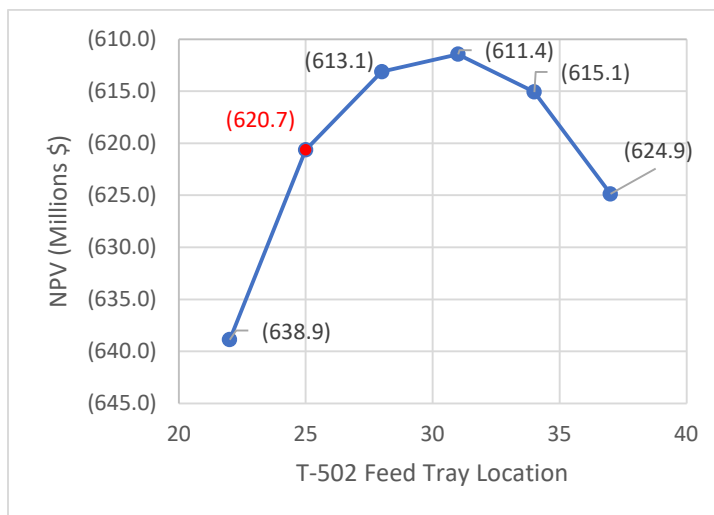
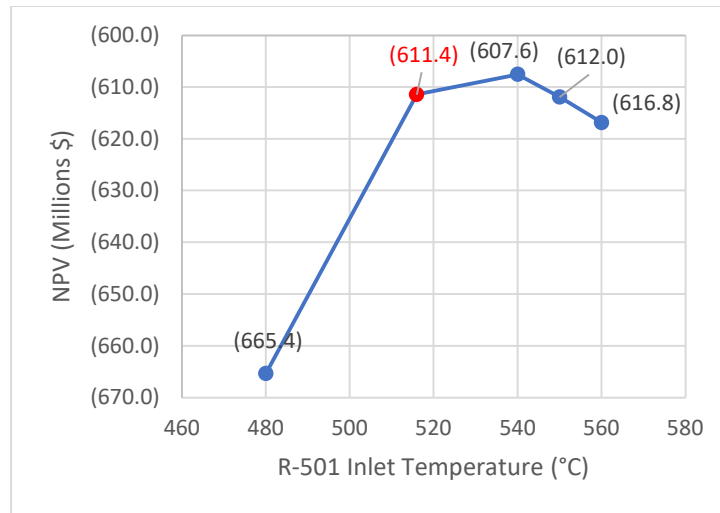


Figure 15: NPV vs T-502 Feed Tray Location

## Review of Selected Variables

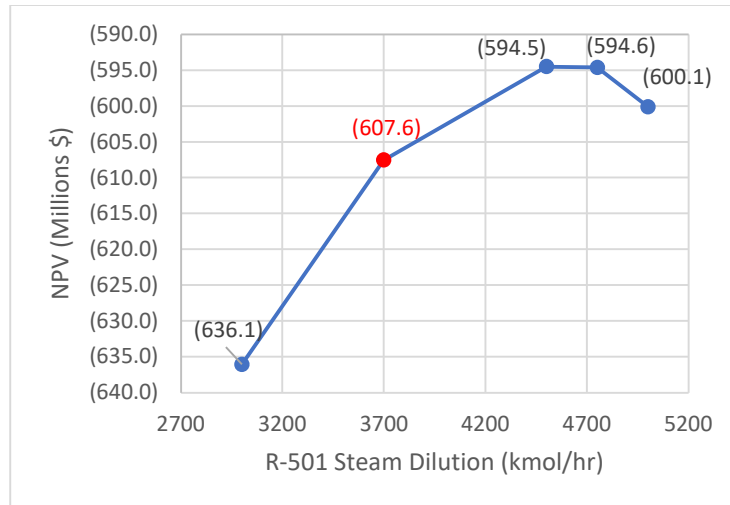
Several variables were reviewed after completing the first round of optimization. Inlet temperature to R-501, steam dilution to R-501, and the temperature of the feed to the three-phase separator.

The temperature of R-501 was tested once more with larger deviation from the base case values. Further savings were found by increasing the temperature from 516°C to 540°C.



*Figure 16: NPV vs R-501 Inlet Temperature*

The steam dilution was also tested for any additional savings and improvement was found by adjusting the from 3700 kmol/hour to 4500 kmol/hour of steam.



*Figure 17: NPV vs R-501 Steam Dilution*

As mentioned in the pre-separation section of the paper, the pre-separation stage was previously only investigated to 25°C. It was later realized that 15°C could be achieved using RW and an analysis was completed. Moving from 25°C to 15°C improved NPV by ~\$21 million to bring NPV to \$(586) million. It should be noted that RW has an approach temperature of 5°C and 10°C is the true limit for the process stream temperature for using RW utility. (Turton, Shaeiwitz, Bhattacharyya, & Whiting, 2018) This was not known until after completion of the analysis and was not investigated but likely presents further opportunity for NPV improvement.

The various heat exchangers in the process were then sized using zone analysis. This resulted in an NPV increase of about \$3 million to ~\$(583) million. Any further analysis after this point used zone analysis and is reflected in the NPV calculation.

### **Compressor Optimization**

The fuel gas compressor in the base case used a compression ratio that exceeded heuristic recommendations. (Turton, Shaeiwitz, Bhattacharyya, & Whiting, 2018) Due to this high ratio, the compressor was expensive to purchase and operate. To address this, an intercooler and an additional compressor were added to reduce the per stage compression ratio and to approximate

isothermal compression. This allows for improvement as isothermal compression is more efficient than isochoric compression at compression ratios greater than 2 to 4. (Turton, Shaeiwitz, Bhattacharyya, & Whiting, 2018) This change allows for proper compression of the fuel gas while decreasing the cost. Through the addition of the second compressor and intercooler, the NPV was increased by \$7 million to \$(579) million.

### **Final Tower Material of Construction Change**

After review of material compatibility matrices and discussion with the management team. The decision was made to move from stainless steel towers to carbon steel towers. This improved the overall NPV by an additional \$40 million to \$(539) million. Though, there are no noted issues with the use of carbon steel in these towers, a material expert should be further consulted on this decision.

### **Heat Integration**

Heat integration uses process streams to either heat or cool a stream instead of using utilities. The primary location for heat integration in the process was to use the reactor effluent in E-501 to preheat the reactor feed stream. This also serves to cool the reactor effluent and further reduced the cost of utilities. This optimization improved the NPV to \$(534) million.

### **The Optimized Design Description**

After the completion of the optimization process, there were little changes to the overall process layout. The stream from the reactor effluent was fed into heat exchanger E-501 reducing the utility usage. The addition of heat exchanger E-510 with refrigerated water reduced the outlet temperature of the pre-separation. Finally, compressor C-502 and heat exchanger E-511 were added. Compressor C-502 was added to reduce the per stage compression ratio. The

heat exchanger was used as an intercooler between the two compressors to help approximate isothermal compression. A PFD of the final process with changes from base case in red is available in Appendix B.

### **Community, Environmental and Government Considerations**

This project is also dependent on a number of key issues outside of the operations of the plant. There are many things to consider such as community support for heavy industry, environmental considerations, and the ability to gain key advantages from local and national governments. With regards to community support, movements such as “Not in My Backyard” (NIMBY) have been instrumental in blocking key development projects in a number of major cities. This is important as it may present challenges to development of Unit 500 as well as any relevant infrastructure that will be needed for Unit 500’s successful operation. Conversely areas that would benefit heavily from the economic impact of these operations may be highly willing to accept Unit 500’s build plans. Similarly local environmental regulations should be considered when deciding the location of Unit 500 as the nature of the process is within the realm of chemical processing. A variety of the chemicals that occur in the process are harmful to the environment if containment is lost. This will likely limit the plant to a less populated areas and those with poor environmental protections. Finally, the willingness of local governments to support Unit 500’s construction and continued operation should be considered. If the project is opposed, it could make implementation and continued operation unlikely. Support for the project could be highly beneficial and reduce the tax burden on the project and aid in the approval of necessary infrastructure improvements and projects necessary for successful operation.

The availability of styrene both now and in the future should also be investigated to ensure that there will be enough to meet corporate needs if the decision is made to purchase

rather than build. Similarly, an analysis should be performed involving the liabilities associated with plant ownership.

### **Process Safety Considerations**

Though early in the design process, safety should be considered. Noted issues include, but are not limited to, flammable materials, dangerous chemicals, high pressure associated with the injected super-heated steam, high temperature in R-501 and R-502, vacuum pressure, and rotary equipment. Further analysis is required to ensure proper understanding of process safety if the project proceeds. These early concerns will mainly be addressed with proper design practices. Equipment should include all necessary flame suppression equipment and explosion venting. Care should be taken to eliminate possible ignition sources. Equipment and piping should be properly grounded and bonded. Exposure to the process chemicals should be limited and levels monitored through the process environment. Immediately address any loss of containment and conform to any reporting protocols. Controls should be implemented to ensure control of temperatures and pressures. Pressure and vacuum relief systems should be added, though care should be taken to not introduce oxygen as the components are flammable. Also, proper guarding and protection surrounding all pumps, drives, and rotary equipment should be incorporated in the design. Standard operating procedures should be developed, and training planned for all site personnel. Finally, proper PPE should be selected to protect operators from exposures and general workplace injury.

### **Final Report Recommendations**

After completing the optimization of Unit 500. The Unit 500 NPV is \$(534) million and the production cost of styrene is \$2,035 per metric ton. As mentioned previously, the market price of styrene is \$1,598 per metric ton. It is recommended that any issues mentioned in the



optimization above be addressed, other options be considered, and a market risk analysis be performed, while halting major work on Unit 500.

## Fluidized Bed Reactor Analysis

Analysis was completed on a fluidized bed reactor (FBR). This reactor used the previously described reactions, R1-R4, and respective rate equations for Unit 500. The objective of this reactor was to convert ethylbenzene to styrene while maximizing the achieved selectivity of ethylbenzene to styrene. This analysis was completed using PRO/II Process Simulator. This analysis was completed using constraints given in the table below.

Table 1: Tested Constraints of Reactor

<b>Constraints</b>	<b>Limits for Constraint</b>	<b>Units</b>
L/D Ratio	2 to 10	
Inlet Feed Pressure	0.75 to 5	Bar
Inlet Feed Temperature	300 to 700	°C

The stream entering the reactor was composed of the following components:

Table 2: Reactor Feed Composition

<b>Components</b>	<b>Flow (kmol/hr)</b>
H <sub>2</sub> O	8000.00
Ethylbenzene	512.70
Styrene	1.20
Benzene	1.80
Toluene	2.13
Total	8517.83

## Background Information

Fluidized bed reactors operate by using fluid velocity to suspend catalyst in a fluidized state. Once the fluid velocity is sufficiently high, such that the drag force applied by the fluid equals the gravitational force, the particles are said to be fluidized. This fluidization allows for greater heat transfer than many other reactors, such as packed bed reactors and plug flow reactors, as the particles are more capable of carrying thermal energy than vapor. This allows the fluidized bed reactor to operate at nearly isothermal conditions. The increase in heat transfer prevents runaway exothermic reactions and prevents endothermic reactions slowing their rates through consumption the available thermal energy. Fluidized beds also lack the associated downtime of packed bed reactors as FBRs require large amounts of time to ensure proper catalyst filling. However, fluidized beds are prone to loss of catalyst due to fluidization, poor scalability, and reduced mass transfer due to bubble creation in the operation of the FBR. (Cocco, Karri, & Knowlton, 2014)

## FBR Optimization

The FBR was modeled in PRO/II. To model bubbling in the reactor system, a 10% bypass was used. Bubbling within the reactor limits conversion to 90%. Besides the constraints mentioned previously in table 1, the conversion should be at least 5% and the superficial gas velocity should be limited to between 3 and 10 times the minimum fluidization velocity,  $u_{mf}$ .  $u_{mf}$  may be calculated using equation 1, the Wen and Yu Correlation:

$$Re_{p,mf} = \frac{u_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408Ar]^{0.5} - 33.7 \quad (1)$$

where  $d_p$  is catalyst particle diameter,  $\rho_g$  is the gas density,  $\mu_g$  is the gas viscosity, and  $Ar$  is the Archimedes number. The Archimedes number is described by equation 2:

$$Ar = \frac{d_p^3(\rho_s - \rho_g)\rho_g g}{\mu_g^2} \quad (2)$$

where  $\rho_s$  is the catalyst density, and  $g$  is acceleration due to gravity.

Using these equations, constraints, and the optimizer function in PRO/II, the analysis for the FBR was completed. The optimum conditions for this system are given in the table below:

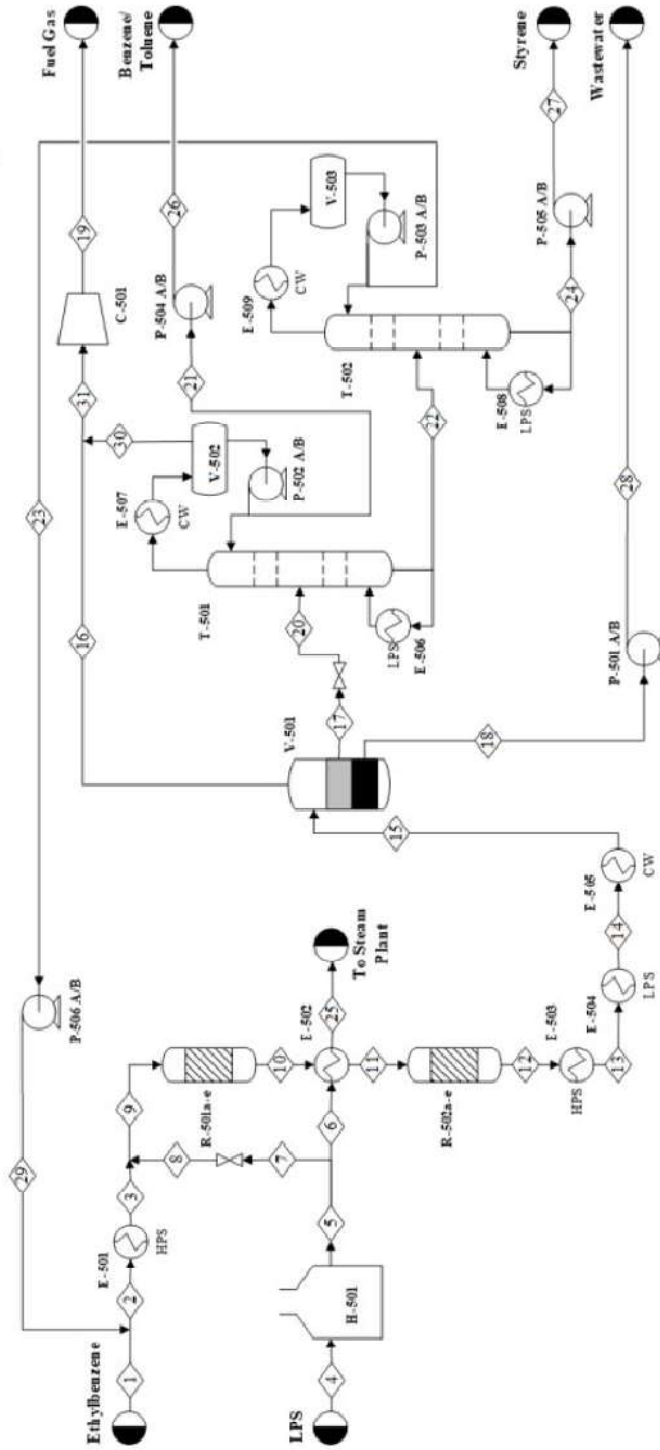
Table 3: Optimized Conditions

Condition	Value	Unit
Feed Temperature	488	°C
Feed Pressure	3.6	Bar
Reactor Volume	196	m <sup>3</sup>
Reactor L/D	2	
Inlet Velocity	1.9	m/s
Outlet Velocity	2.3	m/s
Minimum Fluidization Velocity	0.4	m/s

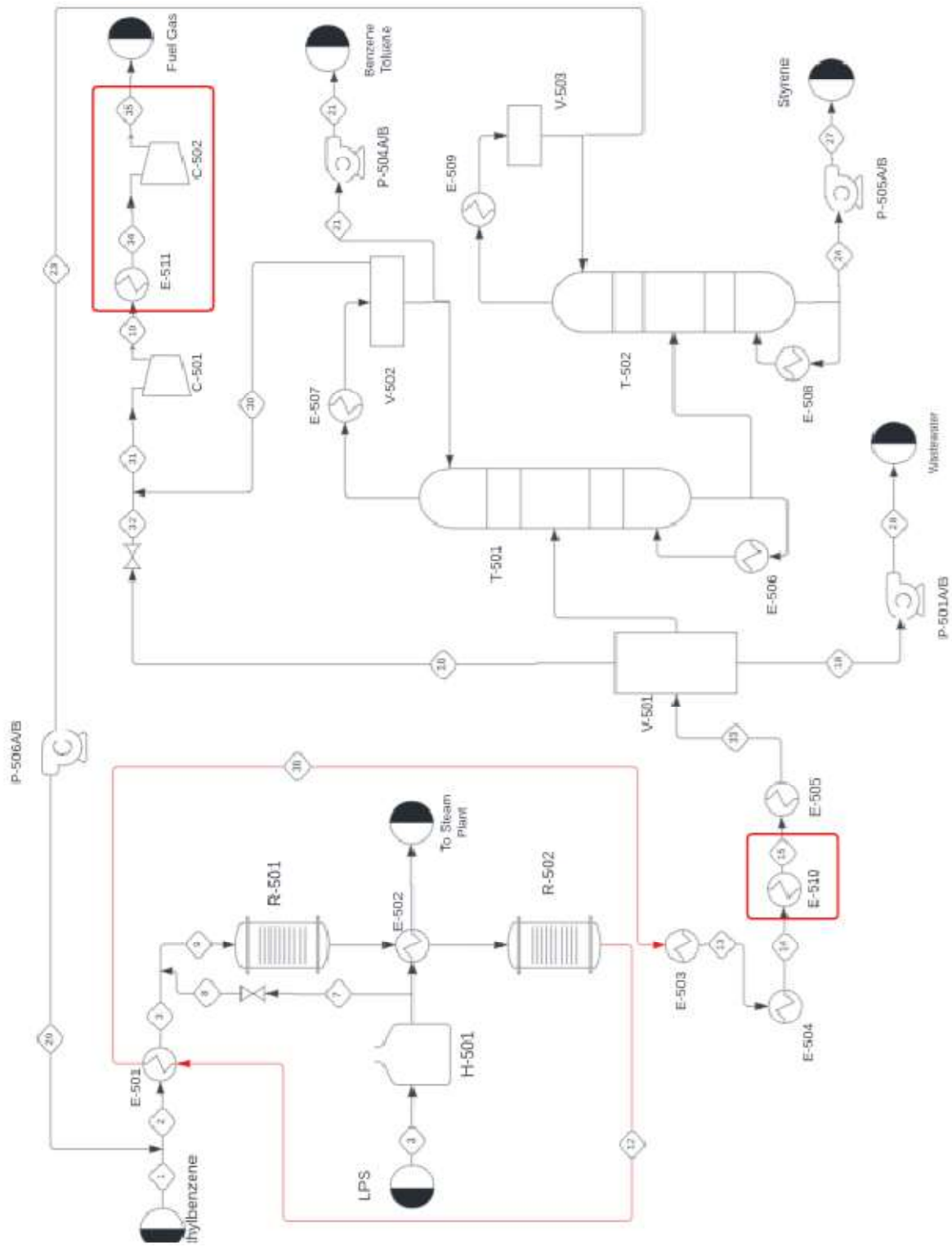
The selectivity was maximized to 12.0 at the minimum required conversion within the reactor. This is in agreement with analysis previously completed on Unit 500 as it was noted that selectivity and conversion were generally in opposition to one another for this reaction scheme. While this selectivity is much greater than the optimized overall selectivity from the analysis of Unit 500, 2.25, and will greatly reduce the fresh ethylbenzene that must be feed to achieve the required. However, it should be noted that the FBR's conversion is 5% compared to 28%. This will have implications on the size of downstream unit operations as it will require a very large recycle to produce the required rate of styrene. Outside of the implications for the tower, analysis would need to be completed to price the reactor, the replacement schedule of catalyst, the internal heat exchanger utility costs, and the implications of this change for the separation

section of Unit 500. While there is likely to be an increase in costs associated with the reactor section of Unit 500, savings in capital costs from the separation section and improvement in raw material utilization warrant further investigation into the financial impacts of FBRs on Unit 500.

# Appendix A: Base Case PFD



## Appendix B: Updated PFD



## Appendix C: Updated Stream Tables

Refer to Excel Workbook “Unit 500 Economic Model” for improved readability of Appendices C-F.

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12
Temperature (°C)	136.00	106.12	217.00	158.98	812.50	812.50	812.50	811.63	540.54	513.96	555.00	538.86
Pressure (kPa)	230.00	230.00	210.00	600.00	565.00	565.00	565.00	210.00	210.00	194.16	179.16	167.06
Vapor Mole Fraction	0.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Total Flow (kg/h)	19351.63	65419.05	65419.05	136134.55	136134.55	55065.79	81068.76	81068.76	146487.81	146487.29	146487.29	146487.29
Total Flow (kmol/h)	183.00	616.98	616.98	7556.62	7556.62	3056.62	4500.00	4500.00	5116.98	5199.67	5199.67	5258.84
Component Flows												
Water	0.00	0.00	0.00	7556.62	7556.62	3056.62	4500.00	4500.00	4500.00	4500.00	4500.00	4500.00
Ethylbenzene	179.34	611.76	611.76	0.00	0.00	0.00	0.00	0.00	611.76	517.96	517.96	437.73
Styrene	0.00	1.22	1.22	0.00	0.00	0.00	0.00	0.00	1.22	75.40	75.40	121.83
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	63.09	63.09	88.45
Benzene	1.83	1.83	1.83	0.00	0.00	0.00	0.00	0.00	1.83	10.34	10.34	23.09
Toluene	1.83	2.17	2.17	0.00	0.00	0.00	0.00	0.00	2.17	13.27	13.27	34.33
Ethylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.51	8.51	21.26
Methane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	11.10	11.10	32.16

Stream No.	13	14	15	16	17	18	19	20	21	22	23	24
Temperature (°C)	270.00	180.00	15.00	15.00	15.00	15.00	119.59	15.02	50.15	122.75	90.80	123.60
Pressure (kPa)	152.06	137.06	107.06	107.06	107.06	107.06	104.88	60.00	46.00	66.00	25.00	55.00
Vapor Mole Fraction	1.00	1.00	0.03	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
Total Flow (kg/h)	146487.84	146487.84	146487.84	1406.23	64106.11	80975.49	1817.66	64106.11	5061.89	58631.60	46067.42	12564.18
Total Flow (kmol/h)	5258.85	5258.85	5258.85	143.13	621.13	4494.58	151.71	621.13	57.88	554.61	433.98	120.63
Component Flows												
Water	4500.00	4500.00	4500.00	2.29	3.22	4494.48	4.86	3.22	0.59	0.00	0.00	0.00
Ethylbenzene	437.74	437.74	437.74	0.68	437.03	0.03	0.75	437.03	4.30	432.66	432.42	0.24
Styrene	121.83	121.83	121.83	0.12	121.71	0.00	0.12	121.71	0.10	121.61	1.22	120.39
Hydrogen	88.45	88.45	88.45	88.33	0.12	0.00	88.45	0.12	0.00	0.00	0.00	0.00
Benzene	23.09	23.09	23.09	0.39	22.69	0.00	2.75	22.69	20.33	0.00	0.00	0.00
Toluene	34.33	34.33	34.33	0.17	34.13	0.03	1.46	34.13	32.50	0.34	0.34	0.00
Ethylene	21.26	21.26	21.26	19.61	1.64	0.00	21.20	1.64	0.05	0.00	0.00	0.00
Methane	32.16	32.16	32.16	31.54	0.58	0.04	32.11	0.58	0.00	0.00	0.00	0.00

Stream No.	25	26	27	28	29	30	31	32	33	34	35	36
Temperature (°C)	700.00	50.18	120.95	15.01	93.04	50.00	18.40	14.88	40.00	88.66	204.00	434.60
Pressure (kPa)	550.00	200.00	200.00	200.00	230.00	46.00	46.00	46.00	122.06	104.88	239.13	167.06
Vapor Mole Fraction	1.00	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.03	1.00	1.00	1.00
Total Flow (kg/h)	55065.79	5061.89	12564.18	80976.69	46067.42	411.42	1817.66	1406.23	146487.84	1817.66	1817.66	146487.29
Total Flow (kmol/h)	3056.62	57.88	120.63	4494.65	433.98	8.58	151.71	143.13	5258.85	151.71	151.71	5258.84
Component Flows												
Water	3056.62	0.59	0.00	4494.55	0.00	2.57	4.86	2.29	4500.00	4.86	4.86	4500.00
Ethylbenzene	0.00	4.30	0.24	0.03	432.42	0.07	0.75	0.68	437.74	0.75	0.75	437.73
Styrene	0.00	0.10	120.39	0.00	1.22	0.00	0.12	0.12	121.83	0.12	0.12	121.83
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.12	88.45	88.33	88.45	88.45	88.45	88.45
Benzene	0.00	20.33	0.00	0.00	0.00	2.36	2.75	0.39	23.09	2.75	2.75	23.09
Toluene	0.00	32.50	0.00	0.03	0.34	1.29	1.46	0.17	34.33	1.46	1.46	34.33
Ethylene	0.00	0.05	0.00	0.00	0.00	1.59	21.20	19.61	21.26	21.20	21.20	21.26
Methane	0.00	0.00	0.00	0.04	0.00	0.58	32.11	31.54	32.16	32.11	32.11	32.16



## Appendix D: Utility Tables

Exchanger	E-501	E-502	E-503	E-504	E-505	E-506	E-507	E-508	E-509	E-510	E-511
In	hps		bfw	bfw	RW	lps	CW	lps	CW	CW	CW
Out	bfw		hps	lps	RW	bfw		bfw	CW	CW	CW
Temp (°C)	254	812.5	115	115	5	160	30	160	30	30	30
Pressure (Barg)	41	4.63675	0.68675	0.68675	1.01	5	1.01	5	1.01	1.01	1.01
Rate (kg/h)	21,001	55,066	183	617	-	14,004	399,787	56,589	1,935,193		
Rate (MT/h)	21.00	55.07	0.18	0.62	-	14.00	399.79	56.59	1,935.19		
Rate (MJ/hr)	35577.1	14369.4	51941.4	25878.4	12241.1	29154.3	16633.5	117813	120642.4	255590.4	278.9
Rate (GJ/hr)	35.5771	14.3694	51.9414	25.8784	12.2411	29.1543	16.6335	117.813	120.6424	255.5904	0.2789



# Appendix F: Income Cash Flow

End of Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	
<b>Income Statement</b>																
Revenue	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38	202,915,637.38
Expenses	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09	181,124,654.09
Materials	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)	(136,302,894.21)
Labor	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)	(31,256,674.25)
Other (O+)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)
Waste Treatment (Car)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)
Other (O-)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)	(1,360,511.51)
Net Income	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29
<b>Cash Flow Statement</b>																
Net Income	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29
Depreciation	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)	(7,282,542.86)
Change in Working Capital	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)
Net Cash Flow	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Operating Activities	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29	21,790,983.29
Investing Activities	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)	(14,565,085.63)
Financing Activities	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Net Cash Flow	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
<b>Summary Project Metrics</b>																
MARR	22%	NPV(\$0.00)	(54,660,000)	Payback (Conv)	more than 12 years											
DCF/CR	490.04	4411.26%	(56,211,000)	Payback (Disc)	more than 12 years											

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