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THE DESIGN AND OPTIMIZATION OF AN ETHYLBENZENE PRODUCTION PROCESS

By:

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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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To all mentioned and many unmentioned, thank you for your unwavering support and belief in my potential.

ABSTRACT

Alexander Anthony Koons: The Design and Optimization of an Ethylbenzene Process
(Under the direction of Dr. Alexander Lopez)

Ethylbenzene is a foundational organic compound used as a reactant in styrene production. The objective of this thesis is to present the optimization of the in-house production process of ethylbenzene, aiming to avoid external procurement for the downstream styrene manufacturing facility. The process underlines a strategic approach to enhance the yield and cost efficiency of the production of ethylbenzene. An economic analysis revealed a promising net present value of approximately $57.6 million. This thesis not only proposes a viable route for internal ethylbenzene generation but also discusses optimizing the chemical production processes for enhanced efficiency and sustainability.

TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

SECTION I: INTRODUCTION AND BACKGROUND

(Written Jointly by Optimization Team: Alexander Koons, Allen Chatelain, and Chance Ferrell)

INTRODUCTION

The objective of this project was to design and optimize an ethylbenzene production facility to feed a downstream styrene unit. This facility produces ethylbenzene by the alkylation of benzene with ethylene. The facility's goal is to achieve a production rate of 80,000 tonnes per year with the maximization of the project's net present value (NPV). The resulting ethylbenzene product will have a quality of 99.8 mol% containing less than 2 ppm diethylbenzene (DEB). The base case conditions, modeled to predict the original cost estimate of the project, yielded an NPV of approximately -\$22.7 million. After optimization of the process, the current predicted NPV is \$57.6 million. In consideration of the downstream styrene unit, it is recommended to build this facility rather than buying the required ethylbenzene from another vendor.

ETHYLBENZENE CONTEXT

Ethylbenzene is a colorless, flammable hydrocarbon that is naturally found in coal tar and petroleum [1]. It is primarily used in the production of styrene and synthetic polymers. In 2024, ethylbenzene has a market size of 34.71 million tonnes and is expected to reach 36.80 million tonnes by 2029 [2]. Ethylbenzene is produced via the direct addition reaction between ethylene and benzene:

$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethylbenzene}}{C_6H_5C_2H_5}$$

Reaction 1: Main Ethylbenzene Reaction

A side reaction between ethylene and ethylbenzene produces the impurity DEB which needs to be reduced as much as possible:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2}$$

Reaction 2: DEB Reaction

The DEB, produced in the previous reaction, will react with benzene to produce ethylbenzene:

$$\underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{ethylbenzene}}{2C_6H_5C_2H_5}$$

Reaction 3: Trans-Alkylation Reaction

The benzene feedstock contains toluene, which will react with ethylene to form both ethylbenzene and propylene.

$$\underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{ethylene}}{2C_2H_4} \rightarrow \underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{propylene}}{C_3H_6}$$

Reaction 4: Ethylbenzene Side Reaction

Using the reactions above, an ethylbenzene production facility was developed and optimized to maximize NPV while also meeting the desired specifications [3].

SAFETY CONSIDERATIONS

In the interest of safety, the industrial chemicals that will be found in the process of this facility are listed below along with their potential hazards. Human contact with the chemicals identified in **Table 1** must be limited. Personal protective equipment including steel-toe boots, flame-resistant clothing, hard hats, and safety glasses are to be worn inside the facility at all times. A respirator should be worn if contact with chemicals is necessary.

TABLE 1: PROCESS HAZARDOUS CHEMICALS

Chemical	Hazard
Benzene	Flammable, Skin/Eye Irritant, Carcinogenic, Aspiration Hazard
Diethylbenzene	Flammable, Skin/Eye Irritant, Aspiration Hazard
Ethane	Flammable
Ethylene	Flammable, Carcinogenic
Ethylbenzene	Flammable, Toxic, Aspiration Hazard
Propylene	Flammable
Toluene	Flammable, Skin/Eye Irritant, Reproductive Toxicity, Aspiration Hazard

The most concerning safety hazard associated with this facility is the high temperatures and pressures surrounding the reactors. With the most extreme of the reactors operating at around 2000 kPa and 520°C, there is a risk of loss of containment leading to injury to the personnel or damage to the facility or the surrounding environment. The reactors must be diligently checked for corrosion or leakage; however, the stainless-steel construction of the reactors should limit such cases. High-pressure relief valves should be installed throughout the facility to prevent failures of the pipe and systems. Control systems should also be installed to ensure that the temperatures inside the reactors do not go above the maximum temperature allowed for stainless steel construction and to prevent any runaway reactions that may occur due to the exothermic reactions taking place.

BASE CASE ANALYSIS

The initial base case analysis of the ethylbenzene production facility was completed with an incoming feed of 97 mol% benzene with a balance of toluene, and 93 mol% ethylene with a balance of ethane. The benzene enters the facility at a flow rate of 7,853.4 kg/hr and ethylene enters at 2,842.0 kg/hr. From these given flow rates and knowing the amount of ethylbenzene required to feed the downstream unit, calculations were completed in Microsoft Excel to estimate the process mass balance as well as the cost of equipment, utilities, and other important factors. After performing initial assumptions and calculations, we simulated the facility in Aspen Plus. This facilitated the later optimization of the facility, making it easier to adjust the process. We then developed an economic model based on this Aspen Plus simulation, enabling us to calculate costs when optimizing the process. This Aspen Plus simulation and the economic model predicted an NPV of the project of -$22.7 million over its lifespan. A sensitivity analysis was completed on the base case design to assess the projected areas for optimization which yielded the results as seen in **Figure 1**.

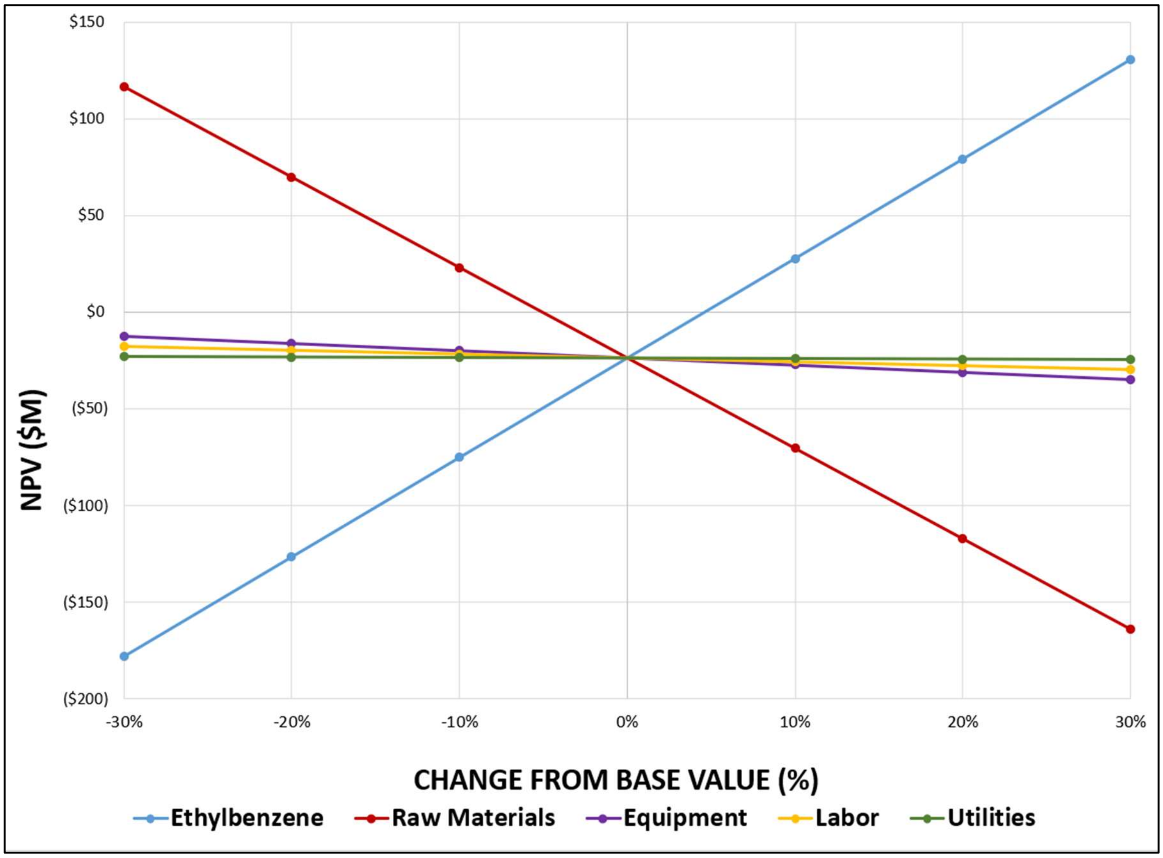


Figure 1: Base Case Sensitivity Analysis

Looking at the slopes of **Figure 1**, the most impactful variables in the process are the cost of raw materials and the revenue from the sale of ethylbenzene. While the prices of raw materials and the product sales price cannot be changed, how efficiently we use the raw materials can be. Optimizing the process will maximize the efficiency of raw material usage and significantly increase the NPV of the facility. Based on the analysis of the base case, we put together an optimization plan to improve the reactors, separations, and heat integration systems of the process.

PROCESS DESCRIPTION

Most ethylbenzene processes produce ethylbenzene for internal consumption within a coupled process that produces styrene monomer. The base case facility produces 80,000 tonnes per year of 99.8 mol% ethylbenzene that is consumed by a downstream styrene facility. A block flow diagram of the process appears in **Appendix A** for a simple overview of the process. As with most ethylbenzene/styrene operations, there is considerable thermal integration shared between the two units. This energy exchange is achieved by the generation and consumption of steam within the two units in alignment with the exothermic nature of the ethylbenzene process and the endothermic nature of the styrene process [3].

The PFD for the base case facility is shown in **Appendix B.** Benzene is combined with recycled benzene in an on-site process vessel (V-301). The mixture is then pumped to a reaction pressure of about 2,000 kPa (20 atm) and sent to a fired heater (H-301) to bring the mixture to a reaction temperature of about 400°C. The preheated benzene is mixed with feed ethylene before entering the first stage of a reactor system containing three adiabatic packed-bed reactors (R-301 to R-303) with interstage ethylene feed addition and cooling. The reaction occurs in the gas phase and is exothermic. The heated effluent from the first reactor is combined with more ethylene and cooled in E-301 to around 380°C before entering the second reactor (R-302), where further reaction takes place. High-pressure steam is produced in E-301 and is sent to the on-site styrene facility. This process repeats with the subsequent reactors, with ethylene addition and cooling, leading to further reaction and steam generation for use in the styrene facility. The effluent stream leaving the final reactor contains products, by-products, unreacted benzene, and small amounts of unreacted ethylene and other non-condensable gases. This stream is then cooled in two waste-heat boilers (E-303 and E-304), which produce both high-pressure and low-pressure steam to be consumed in the on-site styrene facility. The two-phase mixture leaving E-304 goes to a trim cooler (E-305) and then to a two-phase separator (V-302), where the light gases are separated and sent overhead to be sold as fuel gas. The condensed liquid is then pumped to the benzene tower (T-301), where unreacted benzene is extracted as the overhead product and recycled to the front end of the process. The bottom product moves to the ethylbenzene tower (T-302), where ethylbenzene is extracted as the overhead product and directed to the on-site styrene facility. The bottom product from T-302 contains all the DEB and trace amounts of higher ethylbenzenes are mixed with recycled benzene and pass through H-301 before being sent to a fourth packed-bed reactor (R-304), in which the excess benzene is reacted with the DEB to produce ethylbenzene and unreacted benzene. The effluent from R-304 mixes with the liquid entering the waste-heat boiler (E-303), completing the process loop.

SECTION II: OPTIMIZATION

(Written Jointly by Optimization Team: Alexander Koons, Allen Chatelain, and Chance Ferrell)

OPTIMIZATION STRATEGIES

An objective function is the basis of every optimization that provides a numeric value for the process to improve upon. The objective function of this process is to maximize the NPV as it is a key indicator of the profitability and viability of the facility, as a positive value signals a project is profitable over its lifespan. This value is calculated using the minimum acceptable rate of return (MARR) at 12% established for the project to have a baseline of return that the project is expected to make. Next, the design variables and constraints on the process must be identified for the optimization to be effective and realistic. Design variables are factors in the process that can be altered to affect the process such as the reflux ratio of a distillation tower or the outlet temperature of a heat exchanger. The constraints on the system are physical limitations placed on the process and the design variables such as the catalyst poisoning temperature. They provide a maximum (or minimum) value that a design variable can reach.

Using these tools, optimization takes a top-down path to alter the most influential variables first. Topological optimization is the first type considered as it deals with altering the topology of the facility and the arrangement of the equipment. This could include the addition or elimination of unit operations, the elimination of unwanted byproducts, and the integration of heat in the utilities. Following that is parametric optimization. This type of optimization deals with the design variables of the unit operations. Key parametric optimization performed during the optimization of this process includes the inlet temperatures, the reflux ratios in the distillation towers, and pressures at various points in the process. While topological optimization is usually done first, it can be revisited after parametric optimization should the changes warrant significant changes to the topology [4].

Optimization is a continuous and cyclical process that can be streamlined taking the top-down approach until a maximum NPV is found. Based on this value, a decision can be made on whether the process is viable. In the following section, the steps taken to optimize the ethylbenzene production facility are detailed and the results will highlight the viability of this process.

PROCESS OPTIMIZATION STEPS

Our team made several improvements in the ethylbenzene production process to improve the NPV. We initially considered a new catalyst and a change in benzene feedstock due to their byproduct suppression and lower cost respectively. This alteration not only improved our raw material utilization but also lowered material costs. Our team then addressed the issue of the loss of raw materials in the fuel gas, aiming to recapture benzene to maximize feed utilization. Additionally, we carried out reactor optimization by finding the optimum reaction conditions that would lead to better raw material usage, suppression of byproducts, and increased yield. This was followed by an analysis of the process separation units to streamline operations by removing unnecessary equipment and increasing process efficiency. Finally, we conducted a heat integration study to investigate a possible reduction of energy consumption across the plant, hence lowering operational costs. These improvements outline a comprehensive optimization of the ethylbenzene production facility and its development into a more sustainable and efficient chemical production process.

ALTERING FEED AND CATALYST

In the optimization of our ethylbenzene production process, we considered two potential changes from the base case with a focus on their impact on the NPV. The current catalyst in the base case, with a cost of $5/kg and a service life of four years, was compared against a new catalyst option priced at $8/kg with a three-year lifespan. Despite its higher cost and reduced longevity, the new catalyst offered an attractive suppression of DEB. The suppression of DEB production throughout the reactor chain is important as any more than 2 ppm of DEB in the product negatively impacts the downstream styrene production facility. The new catalyst option not only suppressed the production of DEB, but it also allowed for the operation of the reactors at elevated temperatures up to 550°C compared to the previous 500°C.

We tested the new catalyst in our base case design to determine its influence on the process and economics. The catalyst significantly enhanced overall process efficiency, leading to effective suppression of DEB. This suppression suggests a future opportunity to streamline the distillation process, enhancing overall operational efficiency, which will be explored in subsequent sections of our study. The change in catalyst improved the base case NPV from -$22.7 million to -$21.7 million. While the catalyst change had a minimal effect on the NPV, it led us to consider additional optimizations, particularly concerning feed composition.

The second optimization examined the use of a lower grade of benzene feed, which contains 10mol% toluene at a reduced cost of $0.85/kg vs 2mol% toluene at $1.014/kg. The utilization of this feed required a reevaluation of feed rates and tower specifications to ensure that our product met the design requirements of 80,000 tonnes per year, 99.8 mol% ethylbenzene, and no more than 2 ppm DEB. The economic model projected an increase in NPV from our base case NPV of -$21.7 million to $22.5 million.

RECOVERY OF BENZENE

In optimizing the design of the ethylbenzene production facility, a key objective was improving the recovery of benzene in the process. The base case had approximately 7.6 kmol/hr of benzene being lost to the fuel gas stream, which has a value of around $5 million per year. Because of this, we optimized the flash vessel, V-302, and the distillation tower T-301 to maximize the recovery of unreacted benzene in the process.

Our team performed a sensitivity analysis in Aspen Plus, adjusting the inlet temperature of flash vessel V-302 by altering the outlet temperature of heat exchanger E-305. The objective was to understand how temperature variations affect the composition of the fuel gas stream. In the base case, the flash vessel operated at approximately 66°C. However, the analysis revealed that a lower operating temperature resulted in the minimization of benzene lost to the fuel gas. The impact of this change on the NPV can be seen in **Figure 2**. Because we were constrained in the base case by the minimum approach temperature for cooling water, we analyzed the impact of using refrigerated water as the cooling water medium, entering at 5°C and leaving at 15°C, to improve the recovery of benzene. The outlet temperature of E-305 could not be made lower than 15°C due to the refrigerated water exit temperature.

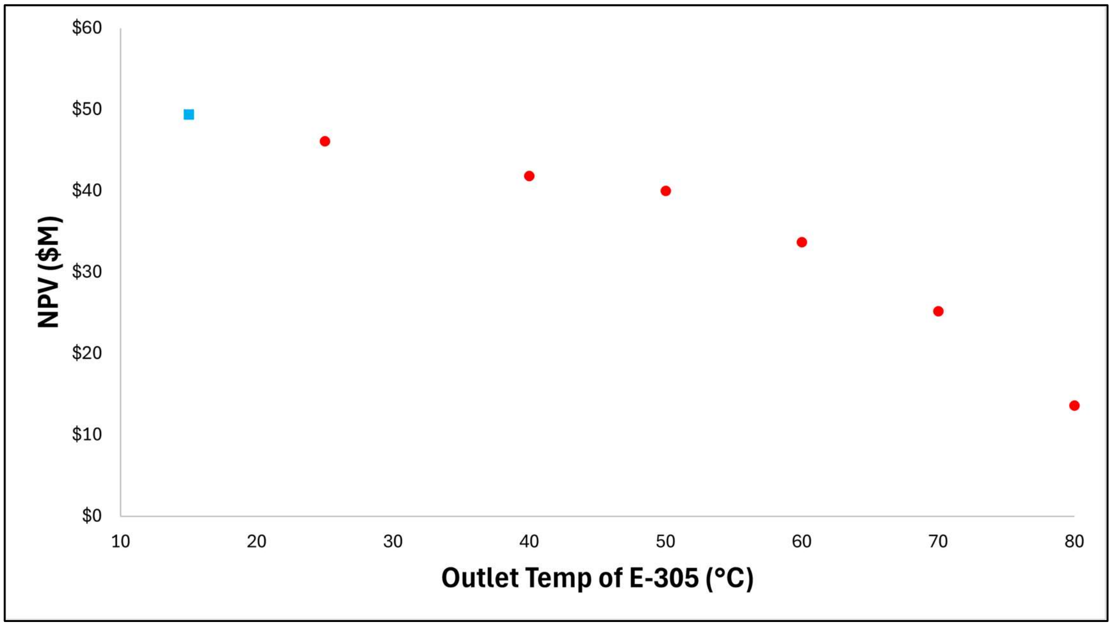


FIGURE 2: NPV VS. OUTLET TEMPERATURE OF E-305

Further modifications included changing E-307, the benzene tower condenser, to use refrigerated water and reconfiguring it from a total to a partial condenser. This improved the separation of the non-condensables from benzene, leading to a reduction in benzene loss to the fuel gas from 7.6 kmol/hr down to 0.9 kmol/hr. Changes in reflux ratio and reboiler duty accommodated the increased recovery of benzene with no change to the sizing of the tower. By recovering the benzene that was previously escaping with the fuel gas, we reduced the raw material input requirements. This reduction was identified in the sensitivity analysis as having a large impact on increasing the project's

NPV, showing the importance of optimizing material use in our process.

The recovery of benzene showed that for every dollar spent on refrigerated water annually, there was a savings of $9.29 per year. While the operational costs associated with refrigerated water were substantially higher—increasing from $33k to $500k annually—the savings incurred from the reduced benzene losses outweighed the increase in utility expenses. The impact of these optimizations increased the NPV from $22.5 million to $49.4 million.

REACTORS

Following the recovery of benzene, we examined our reactor's operating conditions. Given that raw material costs considerably affect the NPV of the process, our strategy focused on optimizing reactor conditions to maximize ethylene conversion while maintaining the high ethylbenzene selectivity. Ethylene conversion is important as unreacted ethylene is lost to the fuel gas due to the volatility of ethylene.

We performed a series of sensitivity analyses in Aspen Plus by varying the inlet temperatures of each reactor in the reactor section by changing the outlet temperatures of H-301, E-301, and E-302, respectively. The goal was to find the most cost-effective balance between ethylene conversion and the selectivity of ethylbenzene over DEB. An important constraint on this optimization was the poisoning temperature of the catalyst at 550°C. We used a safety buffer of 30°C below the poisoning temperature for safe operation while still resulting in high conversion and selectivity. The use of the high-temperature catalyst gave us the ability to explore higher reaction temperatures without compromising the catalyst. We found that an inlet temperature of 440°C was optimal for all reactors—seen in **Figure 3**—because at this point the maximum outlet temperature in the reactor series was 520°C. This optimum outlet temperature was within the safety buffer from poisoning while providing the highest yield and selectivity, so no higher temperatures were considered. High temperatures favor reactions with large activation energies, and by increasing the temperature, we can achieve both alkylation and trans-alkylation reactions simultaneously, so virtually no DEB is produced as a by-product.

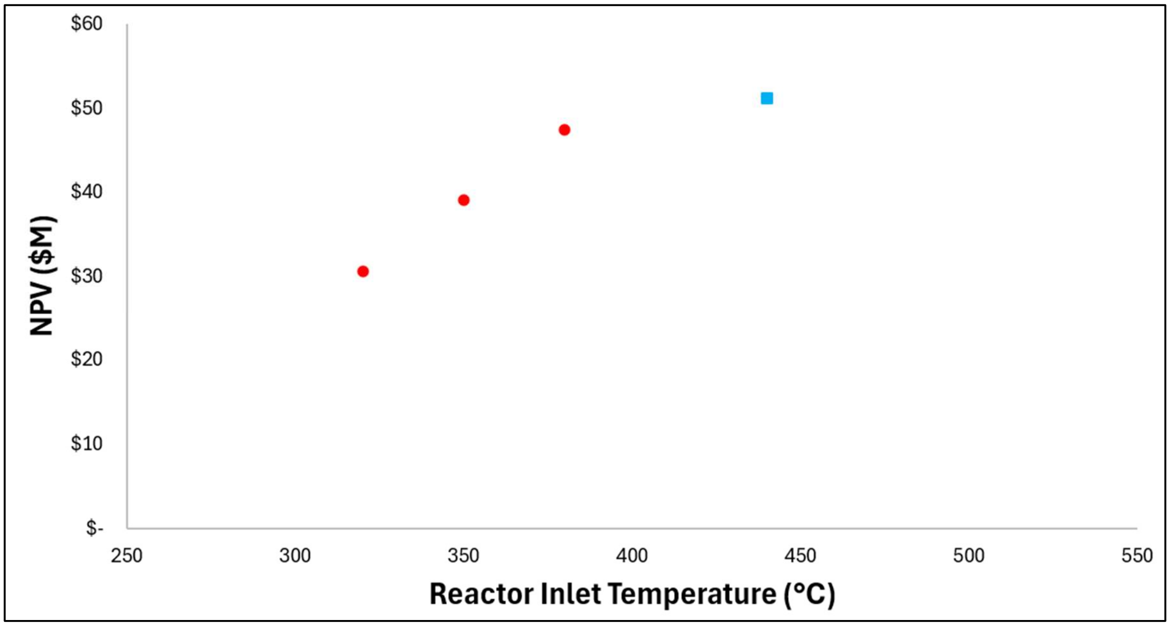


FIGURE 3: NPV VS. REACTOR INLET TEMPERATURE

After we determined an optimal temperature, another sensitivity analysis was performed in Aspen Plus to determine the effect of the reactor length on the conversion of ethylene. We determined that extending the reactor beyond 8 meters yields no additional benefit in conversion rates. Because of this, the optimal reactor length chosen was 8 meters. The results can be seen in **Figure 4**.

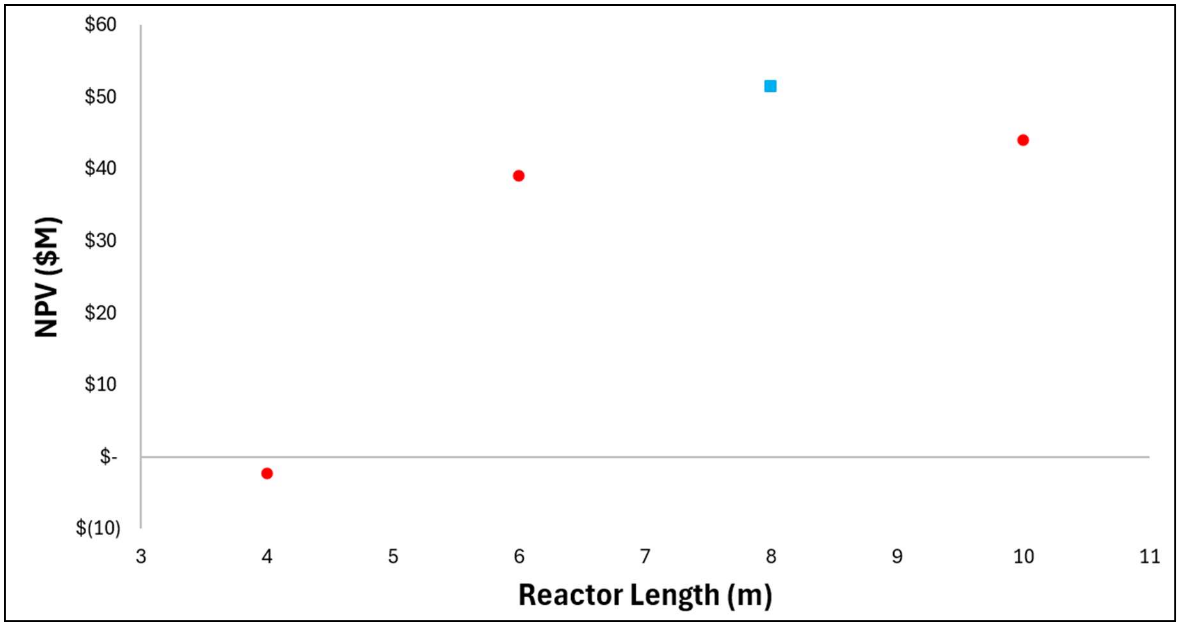


FIGURE 4: NPV VS. REACTOR LENGTH

The optimized reactor configuration resulted in an NPV increase from $49.4 million to $51.2 million with complete conversion of ethylene.

SEPARATIONS

Following the reactor optimization, the next step was to refine the separation section. The adjustments in reactor conditions led to a substantial reduction in DEB production, which rendered the separate DEB recovery system unneeded. Because of this, T-302, R-304, and associated recycle equipment were deemed unnecessary and were eliminated. This topological optimization resulted in capital savings of approximately $945,000. This equipment served only to remove and convert the DEB in the system, and as such, was no longer needed. Removing that equipment improved the NPV from $51.2 million to $57.6 million. This increase is because of the utility cost of running the reboiler and condenser in T-302. The optimized PFD that reflects these changes is in **Appendix C**, along with updated conditions, as seen in red with the updated streams table in **Appendix E**.

We investigated T-301 to determine the impact of the feed tray location on NPV. Upon analyzing the effect of changing the location, we determined that it had minimal impact on NPV. No change was made.

HEAT INTEGRATION

For the final optimization, we analyzed heat integration for our process as it is a critical aspect of reducing utility consumption by recovering waste heat within the system. This involves analyzing heat exchange opportunities to optimize the use of heat and minimize the external energy requirements to reduce operational costs. In our ethylbenzene production facility, the key prospects for heat integration were identified to be the fired heater, H-301, and the first two process coolers after the series reactors, E-303 and E-304. The proposed strategy for improving the energy usage in our process was to utilize the benzene feed in stream three as the cooling utility for either of the coolers to offset the heating duty of H-301. This would result in stream three being preheated by the exothermic reaction and lowering the natural gas consumption.

The implementation of the proposed heat integration resulted in a reduction of heating duty for H-301 from 18,000 MJ/hr to 12,000 MJ/hr. This was the intended result of heat integration; however, this had an unintended consequence. When the cold side utility for E-303 was replaced, that exchanger lost the ability to produce high-pressure steam (hps) which was previously considered an annual credit of $279,000 a year. The reduction in duty only saved $222,000 in natural gas which means that the change resulted in a loss of around $57,000 per year. This hps was intended to be used for the downstream endothermic styrene production facility and it contributed to the income of our current project.

We reviewed the economic impact of this integration which slightly decreased our project's NPV from $57.6 million to $57.4 million. The savings from reducing natural gas usage were insufficient to offset the lost profits from the hps production. Furthermore, heat integration for E-304 was deemed less viable, as this would eliminate the production of low-pressure steam currently valued at $459,000 per year, yielding an even lower NPV than the integration of E-303. While heat integration was a possible opportunity to reduce operational costs, the economic analysis highlighted that the energy created from the exothermic reaction was more valuable for producing steam than it was for reducing heating duty.

SECTION III: INFLUENCE OF REACTION ENGINEERING CONDITIONS

(Written Individually by Alexander Koons to Satisfy Honors College Requirements)

INTRODUCTION TO ISOTHERMAL REACTOR OPTIMIZATION

In addition to the optimization of the gas-phase ethylbenzene production process, it was proposed that a similar process be developed for the production of ethylbenzene using isothermal packed bed reactors. In the highly exothermic gas phase production of ethylbenzene, the decision to use either isothermal or adiabatic packed bed reactors carries implications due to how the different types of reactors manage the heat of the reaction. Isothermal reactors maintain a constant temperature within the reactor, which is achieved by operating them as shell and tube heat exchangers. Tubes packed with catalyst facilitate the reaction while the utility flows within the shell to remove the heat from the exothermic reaction. Isothermal reactors offer control over reaction conditions and allow for minimizing undesirable side reactions such as the formation of DEB, improving the selectivity towards ethylbenzene, and prolonging catalyst life by avoiding thermal degradation.

Adiabatic reactors allow the temperature to rise based on the exothermic nature of the reaction without external heat exchange and are simpler and cheaper to build and operate. They offer energy efficiency advantages in specific applications by utilizing the heat generated by the reaction to drive the process. However, the lack of temperature control can lead to temperature variations within the reactor, increasing the risk of catalyst deactivation and undesirable side reactions.

DESIGN CONSTRAINT AND OBJECTIVES

This section identifies the design constraints used in the isothermal reactor optimization and the specific objectives that this optimization aims to achieve. I varied the inlet feed pressure from 1500 kPa to 2500 kPa and the inlet feed temperature from 300°C to 500°C. I also varied the L/D ratio from 2 to 10 and the reactor volume from 1 m^3 to 5 m^3.

The optimization aimed to improve the selectivity of ethylbenzene to DEB. In improving the selectivity of ethylbenzene, the product purity will be increased, and the production of unwanted DEB will be minimized. I assessed these constraints and objectives through simulation and optimization studies using Aspen Plus. The data found from these simulations provided the foundation to compare the effects of different reactor conditions on the selectivity of ethylbenzene.

METHODOLOGY AND OPTIMIZATION PROCESS

To establish a framework for optimizing the isothermal reactor configuration, I centered the methodology around simulation using Aspen Plus. The starting point involved creating a base case scenario that mirrored the new operating conditions: feed temperatures, pressures, and compositions.

The first step in the simulation required adjusting the feed rates of benzene and ethylene, as well as the specified reflux ratios and distillate-to-feed ratios of both the benzene and ethylbenzene towers. I made these adjustments to align the simulation results to meet the product specifications from the initial base case: producing 80,000 tonnes per operating year of ethylbenzene at 99.8 wt% purity with no more than 2 ppm of DEB. Once these product specifications were met, the resulting simulation conditions were defined as the new base case for the isothermal reactor configuration. This base case then served as the reference point for further analysis, ensuring all optimization efforts were grounded in a scenario that met the pre-existing product specifications.

Using the sensitivity analysis function in Aspen Plus, I varied each of the four decision variables (reactor feed pressure, reactor feed temperature, reactor volume, and reactor L/D ratio). Instead of varying each decision variable independently, I performed the optimization sequence hierarchically. Initially, I adjusted the reactor feed pressure to identify an optimal value, which was then set as a constant for subsequent analyses. This optimal pressure became the new baseline for changing the next variable, the reactor feed temperature. Continuing the cascading approach, the optimal temperature was obtained and then established as a fixed parameter in the base case scenario. The optimization then progressed to the reactor L/D ratio and, subsequently, the reactor volume, each time establishing a new optimal value before proceeding to the following variable.

ANALYSIS OF OPTIMIZATION RESULTS

The initial step in the optimization process focused on reactor inlet pressure, starting with a base case value of 1990 kPa. Upon increasing the pressure incrementally to the upper limit of 2500 kPa, an increase in the selectivity of ethylbenzene over DEB was observed, as depicted in **Figure 5**.

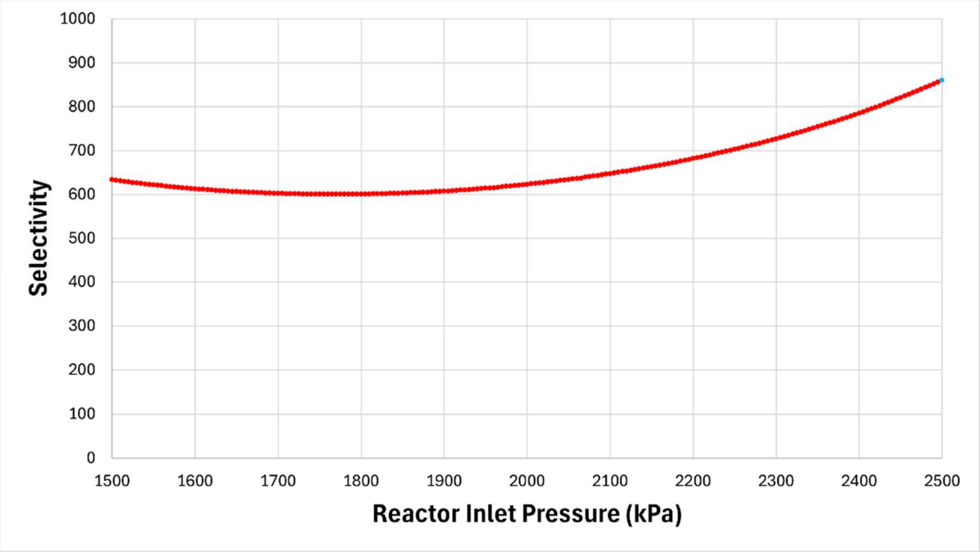


FIGURE 5: SELECTIVITY VS REACTOR INLET PRESSURE

This trend toward higher selectivity at elevated pressures aligns with the principles of reaction kinetics. Increased pressure favors the direct addition reaction between benzene and ethylene due to Le Chatelier's principle because it results in a decrease in the number of moles. Also, the collision frequency between reacting molecules is greater which can lead to a higher reaction rate. At lower pressures, the selectivity also showed a slight increase which can be attributed to the sufficient activation of the benzene and ethylene molecules without the complications introduced by excessive compression. The side reactions that produce DEB and higher polyethylbenzenes are disfavored under high-pressure conditions as these reactions involve the addition of further ethylene molecules to already formed EB, which, due to volumetric and spatial constraints at high pressures, become less likely. Because of this, the optimal pressure of 2500 kPa was selected.

Following the identification of an optimal reactor inlet pressure, the inlet temperature was varied to determine its effect on the selectivity of EB to DEB. The base case operated around 384°C, and an optimal value was approximately 475°C, as seen in **Figure 6**. The observed discontinuity is a direct result of suppression of DEB as the temperature increases. The production of DEB was effectively minimized to the point of being negligible. This appears as a discontinuity in the selectivity data due to how selectivity was calculated. As DEB production approaches zero, the denominator in the selectivity calculation formula also approaches zero. To account for this, a small constant number had to be added to the denominator so that the selectivity could still measure finite results.

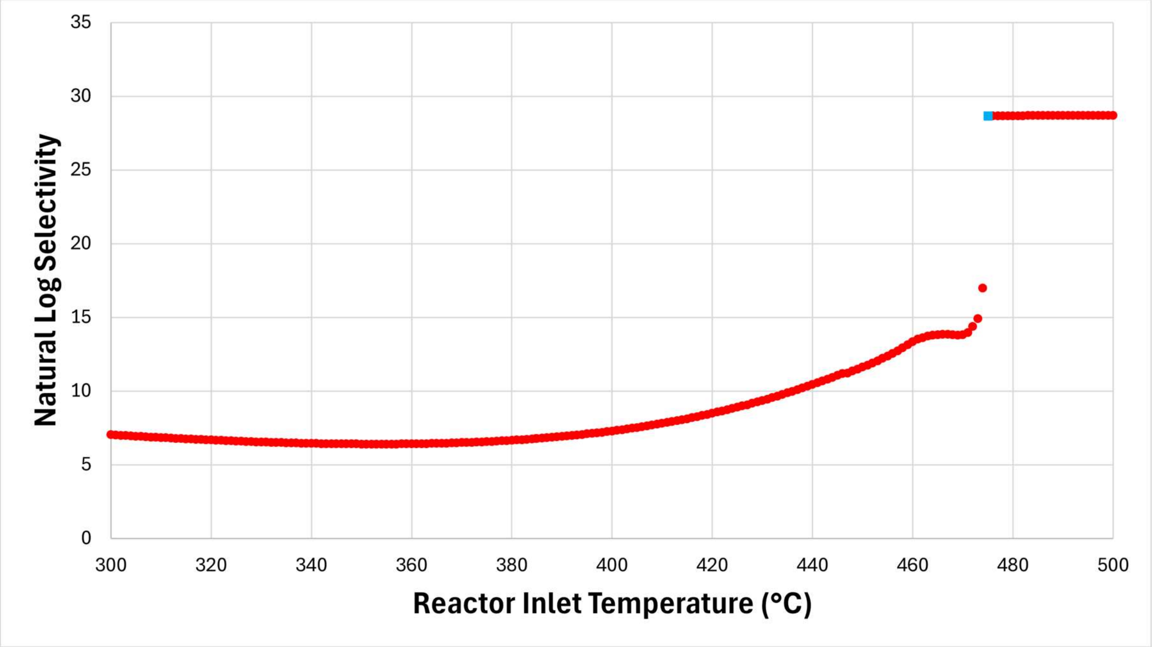


FIGURE 6: SELECTIVITY VS REACTOR INLET TEMPERATURE

In the continued optimization of the isothermal reactor configuration, I varied the length-to-diameter (L/D) ratio to determine its impact on the selectivity of EB to DEB. I kept the reactor volume constant at the base case value of 20 m³ and calculated the diameter from this volume. I then calculated the length using the L/D ratio under consideration. The results, shown in **Figure 7**, reveal an optimal L/D ratio of 5, which corresponds to the base case operation. This L/D ratio demonstrates a balance between the residence time and mixing efficiency within the reactor.

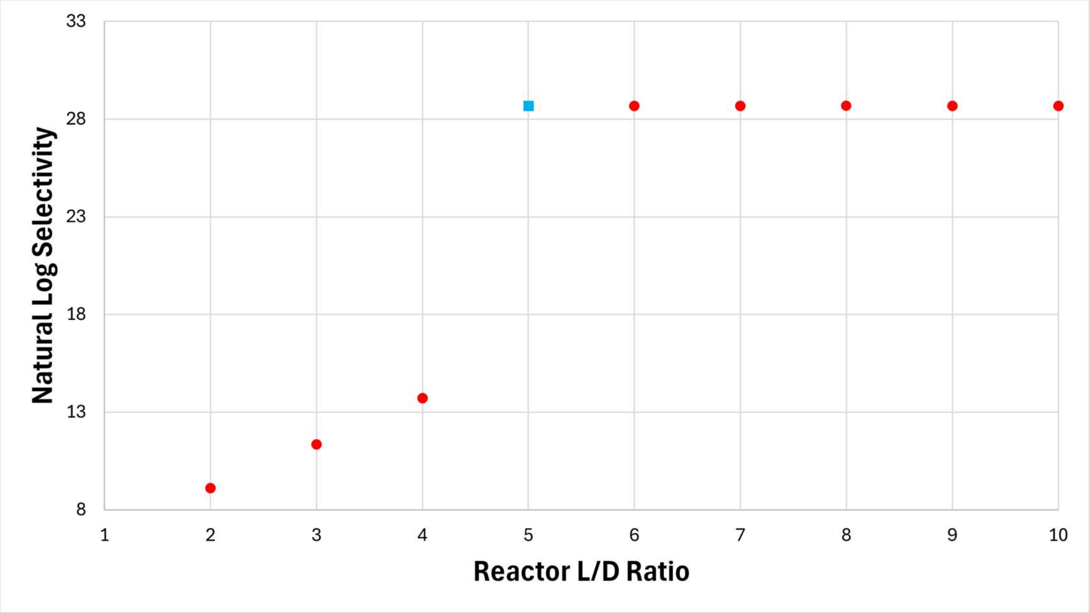


FIGURE 7: SELECTIVITY VS REACTOR L/D RATIO

Finally, I varied the reactor volume while keeping the L/D ratio constant at the optimal value of 5. Initially intending to investigate volumes ranging from 1 to 5 m³, I expanded the analysis to higher volumes to confirm the consistency of the observed trend. The results, displayed in **Figure 8**, identify an optimal reactor volume of 20 m³, consistent with the requirement for sufficient space for the reaction mixture to ensure complete conversion of reactants to the desired products.

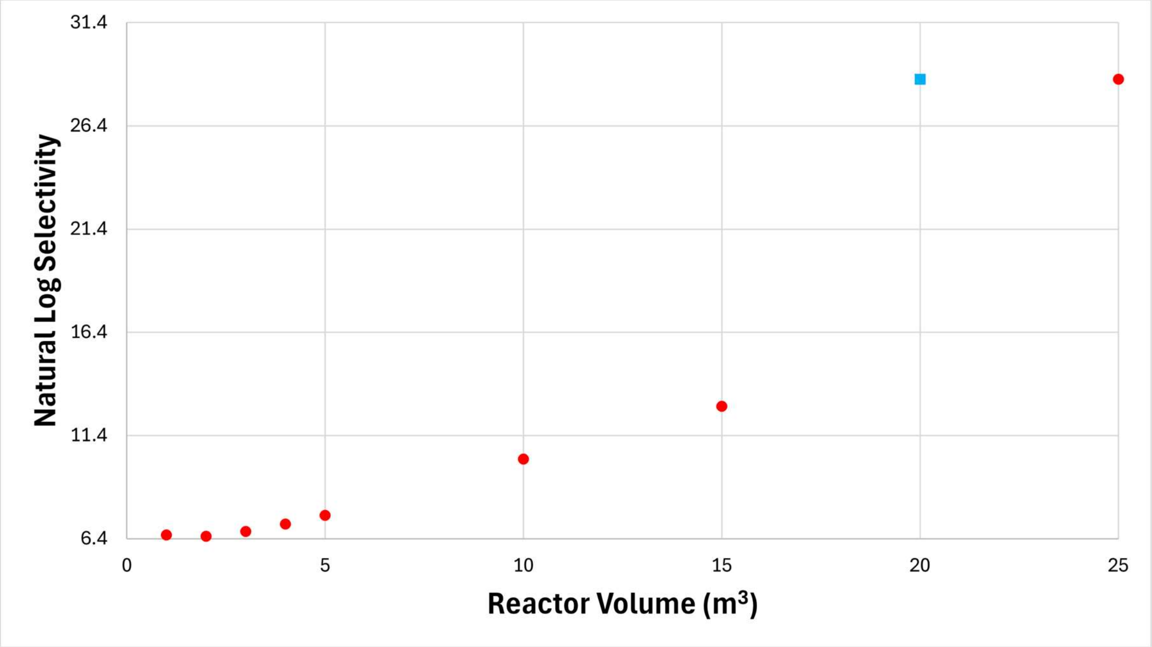


FIGURE 8: SELECTIVITY VS REACTOR VOLUME

The optimization results from both adiabatic and isothermal reactor configurations, as discussed in Section I and the subsequent sections, reveal distinct operational conditions beneficial to optimal performance in each setup. In the adiabatic configuration, the reactor's inlet temperature is regulated more conservatively due to the exothermic nature of the ethylbenzene production reactions. Since the reaction generates heat, there is a corresponding rise in temperature across the reactor's length. The adiabatic reactor's optimal inlet temperature is lower to prevent surpassing the catalyst's maximum temperature of 550°C. The isothermal reactor configuration allows for a higher optimal inlet temperature because the reactor temperature is managed to remain constant despite the heat released by the reaction. Therefore, the system can operate closer to the catalyst's maximum temperature limit, enhancing reaction rates and selectivity without the risk of temperature spikes that could deactivate the catalyst.

SECTION IV: CONCLUSIONS AND RECOMMENDATIONS

(Written Jointly by Optimization Team: Alexander Koons, Allen Chatelain, and Chance Ferrell)

CONCLUSION

After extensive optimization, our team proved the economic viability of the ethylbenzene production facility. The economic analysis projected the NPV at -$22.7 million for the base case design suggesting significant improvements must be made for the project to be recommended. With targeted optimizations across the plant, the project improved its financial outlook by $80.3 million with the current NPV at $57.6 million. The breakdown of the project economics is in **Appendix D,** where the major sources of revenues and costs are outlined. An important takeaway from the economic analysis of the facility is that the Discounted Cash Flow Rate of Return (DCFROR) stands at 33.2%, which exceeds the MARR of 12%, emphasizing the project's strong financial potential. The progression of NPV with each stage of optimization is tabulated in **Figure 9**, where the most impactful changes to the process are the new feed and new catalyst, along with the recovery of benzene lost to the fuel gas.

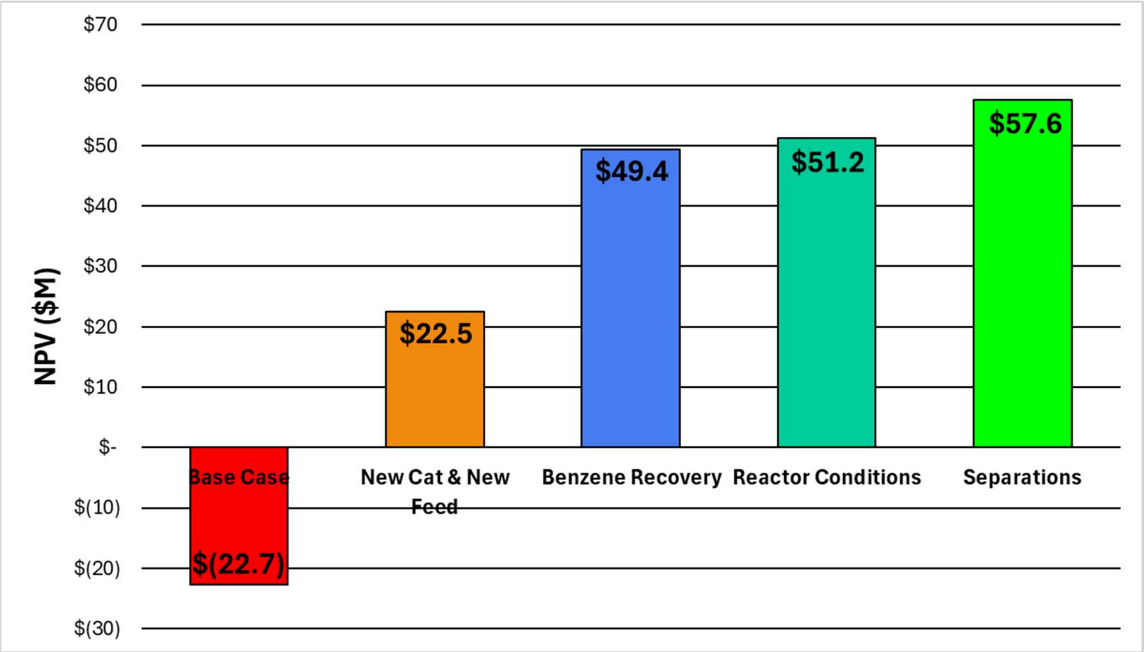


FIGURE 99: OPTIMIZATION SUMMARY

The purpose of this process is to feed the downstream styrene production facility as ethylbenzene is the precursor material for its formation. Producing the ethylbenzene in-house offers significant savings when compared to purchasing the material from an outside source. A conservative estimate to externally procure ethylbenzene would cost around $86.2 million per year and over a billion dollars over the lifespan of the facility. The optimized process offers significant savings to justify the investment in the facility. The improved NPV confirms the project's potential for success after optimization of the base case while providing a cost-effective solution to providing ethylbenzene to the downstream styrene facility. Given these results, our team recommends proceeding with the next stage of detailed engineering for the ethylbenzene production facility.

RECOMMENDATIONS

Our team identified two areas that require further investigation to optimize the ethylbenzene production facility. The first involves expanding heat integration with the downstream styrene production facility. While heat integration within this process did not prove beneficial to the NPV, we expect improvements should the integration involve the styrene process. Utilizing the excess heat generated from the exothermic reaction, heat integration with the endothermic styrene process could prove a more efficient use of energy across both processes and improve both the operational efficiency and the cost of utilities.

The second recommendation draws from the strategies outlined in the separations optimization section for managing fluctuations in DEB levels. The presence of DEB poses a risk to the process as the product specifications limit the amount that can be present to only 2 ppm. Investigating solutions to a process upset to remove this DEB is important to ensure the consistent quality of the product. Analysis of the process during unsteady state conditions would provide a better understanding of the risk of DEB production. These aspects should be closely examined during the next stage of detailed engineering to determine their practicality and impact on the plant’s performance.

REFERENCES

[1] “ToxFAQs for Ethylbenzene.” Centers for Disease Control and Prevention, June 15, 2015.

[2] “Global Ethylbenzene Market Set to Reach 40.56 Million Tons by 2029.” Yahoo! Finance, March 26, 2024.

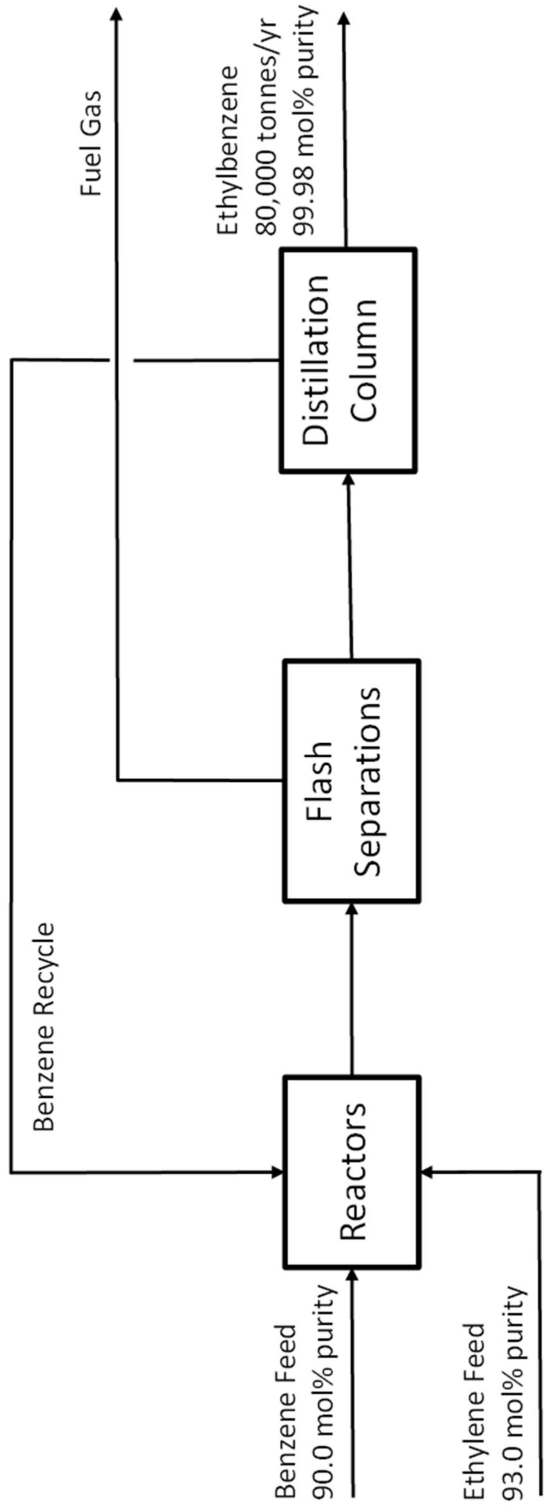
[3] “Production of Ethylbenzene Case Study.” Alexander Lopez, January 2024.

[4] Turton, R., Shaeiwitz, J.A., Bhattacharyya, D., and Whiting, W.B. *Analysis, Synthesis, and Design of Chemical Processes*, 5th Edition, Prentice Hall (2018).

APPENDIX TABLE OF CONTENTS

Appendix A: Base Case BFD

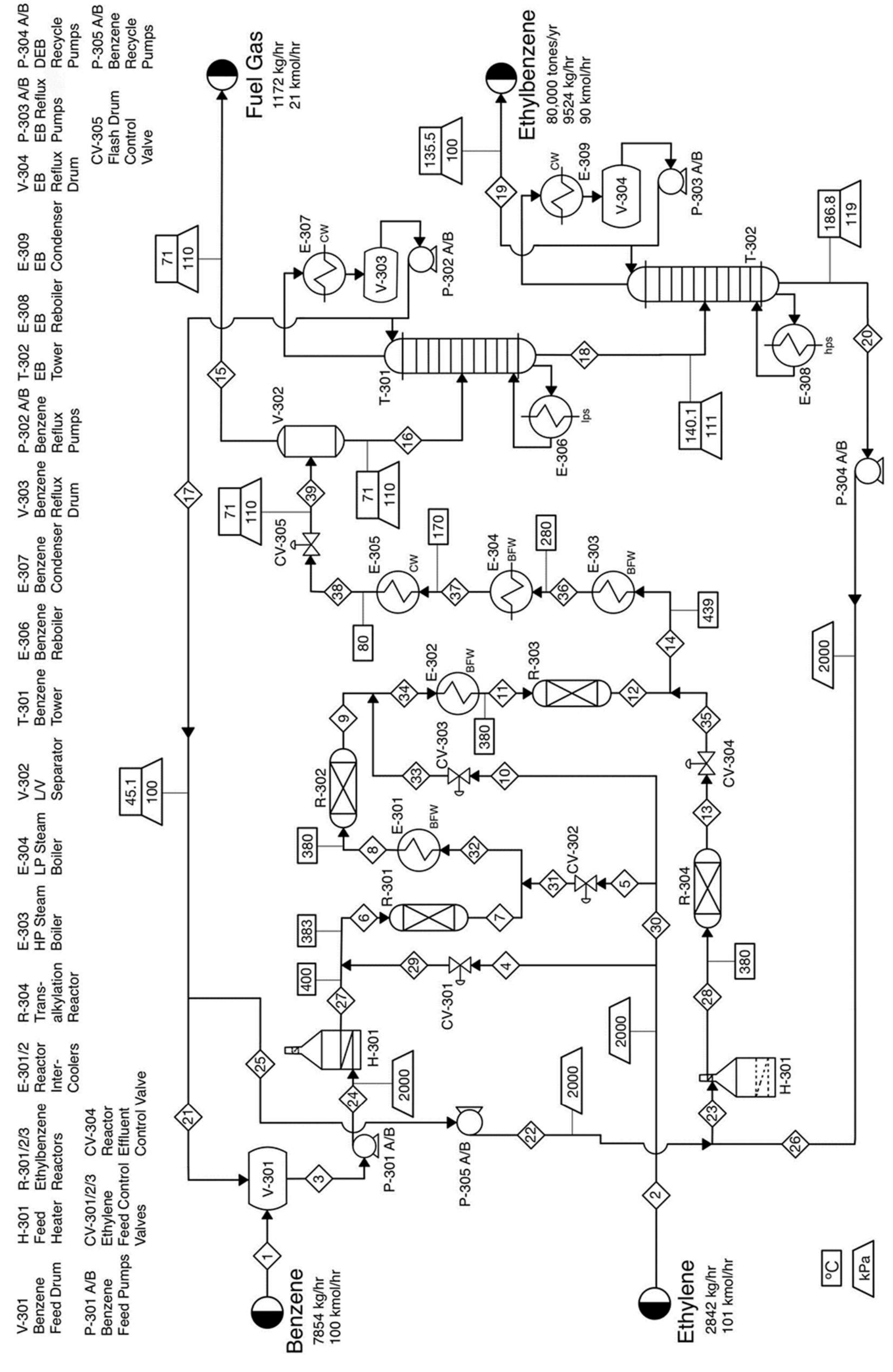
Unit 300 - Ethylbenzene Production Facility BFD



Primary Reactions:

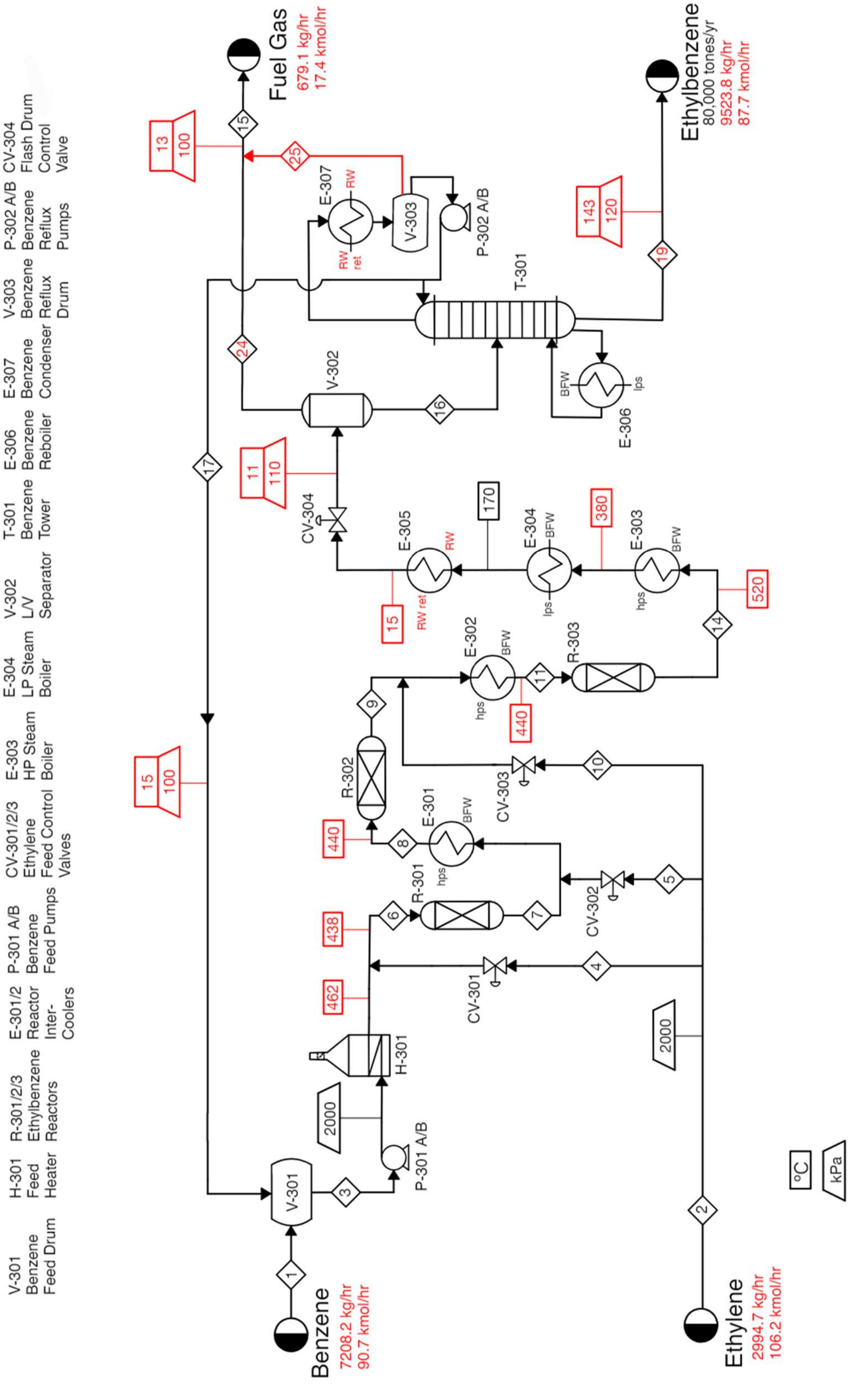
1. Benzene + Ethylene → Ethylbenzene
2. Ethylbenzene + Ethylene → Diethylbenzene
3. Diethylbenzene + Benzene → Ethylbenzene
4. Toluene + Ethylene → Ethylbenzene + Propylene

Appendix B: Base Case PFD



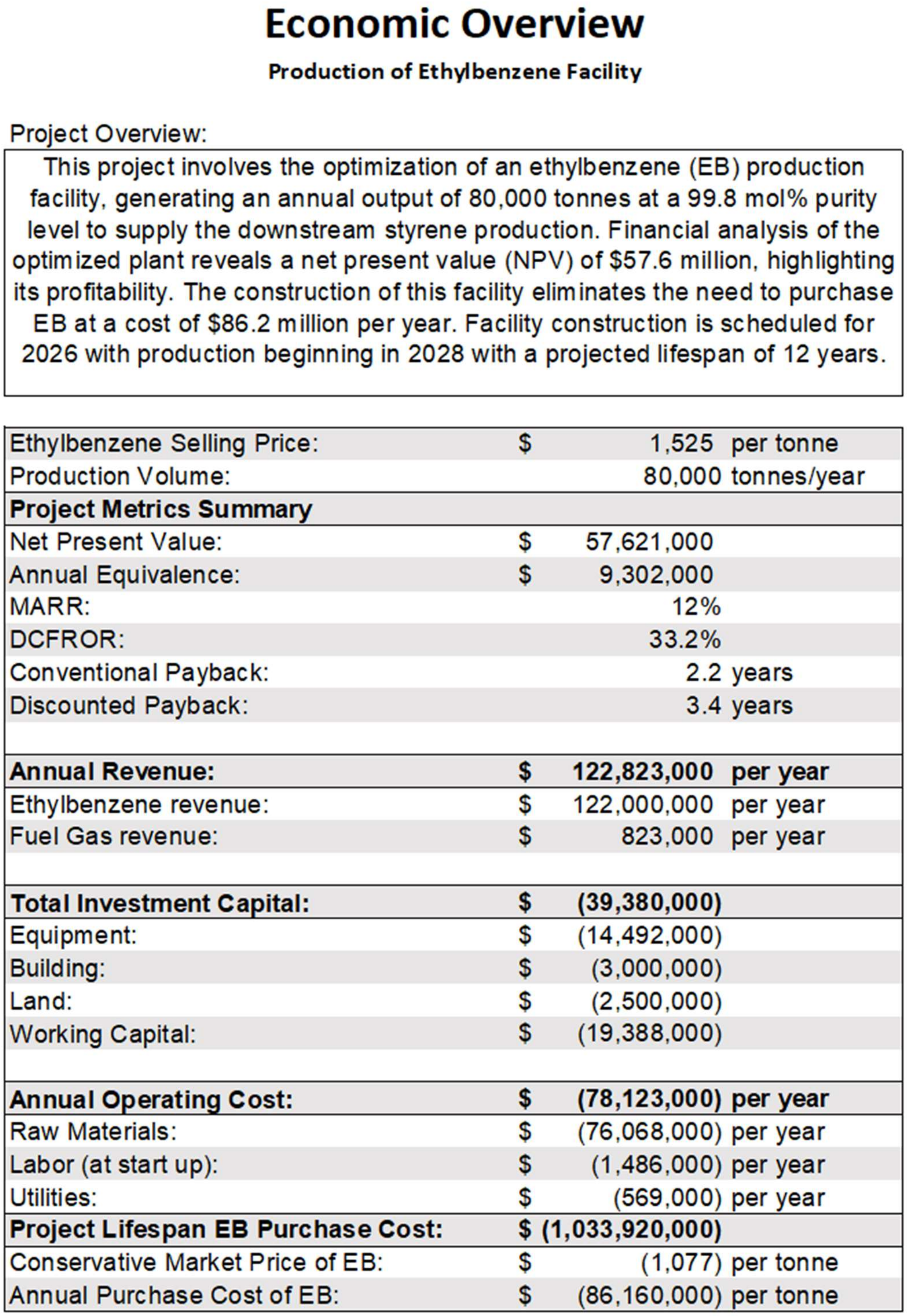
Ethylbenzene Production Facility PFD, Base Case

Appendix C: Optimized PFD



Ethylbenzene Production Facility PFD, Optimized

Appendix D: Economic Overview



Economic Overview

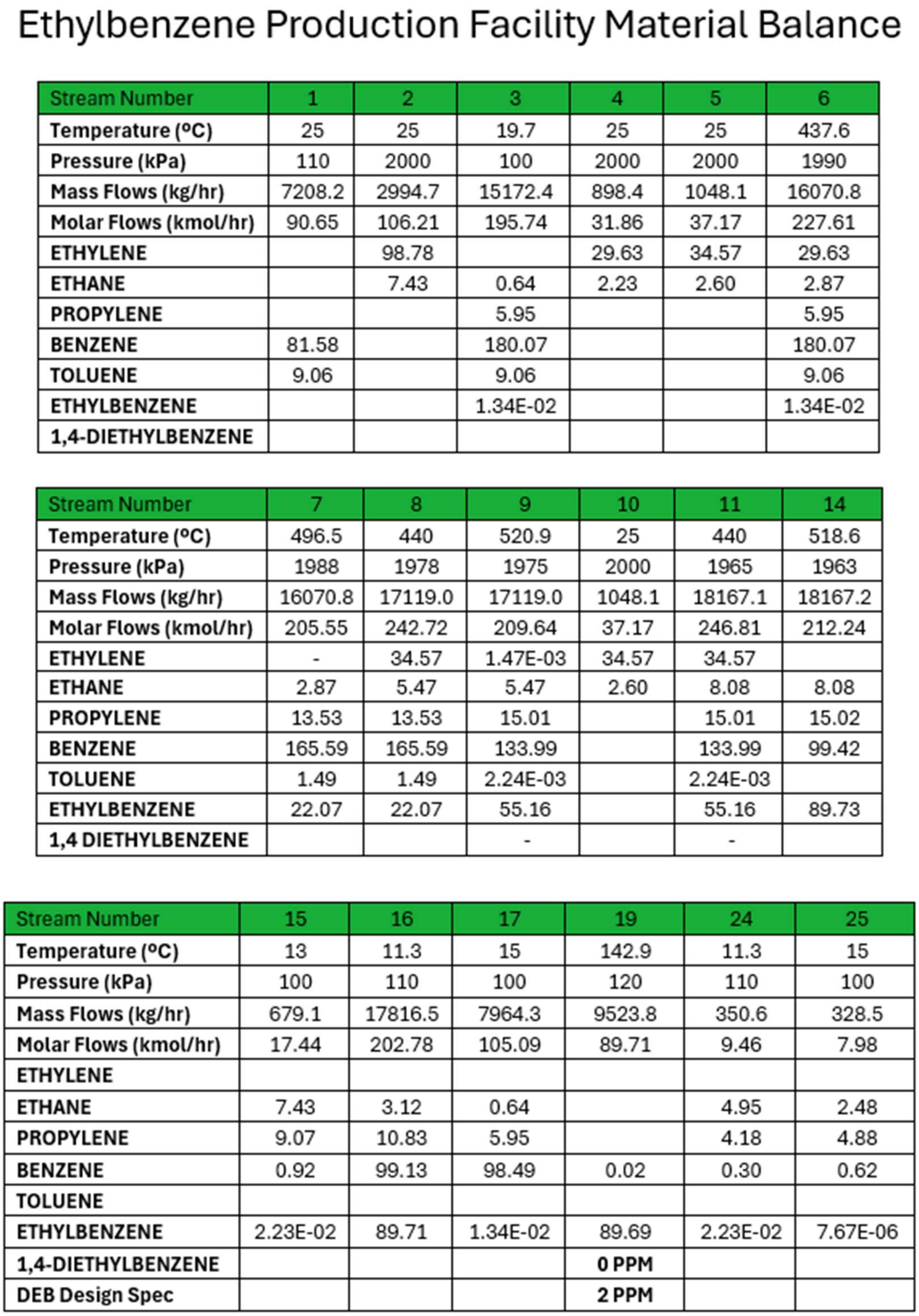
Production of Ethylbenzene Facility

Project Overview:

This project involves the optimization of an ethylbenzene (EB) production facility, generating an annual output of 80,000 tonnes at a 99.8 mol% purity level to supply the downstream styrene production. Financial analysis of the optimized plant reveals a net present value (NPV) of $57.6 million, highlighting its profitability. The construction of this facility eliminates the need to purchase EB at a cost of $86.2 million per year. Facility construction is scheduled for 2026 with production beginning in 2028 with a projected lifespan of 12 years.

Ethylbenzene Selling Price:	$	1,525	per tonne
Production Volume:		80,000	tonnes/year
Project Metrics Summary			
Net Present Value:	$	57,621,000	
Annual Equivalence:	$	9,302,000	
MARR:		12%	
DCFROR:		33.2%	
Conventional Payback:		2.2	years
Discounted Payback:		3.4	years
Annual Revenue:	**$**	**122,823,000**	**per year**
Ethylbenzene revenue:	$	122,000,000	per year
Fuel Gas revenue:	$	823,000	per year
Total Investment Capital:	**$**	**(39,380,000)**	
Equipment:	$	(14,492,000)	
Building:	$	(3,000,000)	
Land:	$	(2,500,000)	
Working Capital:	$	(19,388,000)	
Annual Operating Cost:	**$**	**(78,123,000)**	**per year**
Raw Materials:	$	(76,068,000)	per year
Labor (at start up):	$	(1,486,000)	per year
Utilities:	$	(569,000)	per year
Project Lifespan EB Purchase Cost:	**$**	**(1,033,920,000)**	
Conservative Market Price of EB:	$	(1,077)	per tonne
Annual Purchase Cost of EB:	$	(86,160,000)	per tonne

Appendix E: Optimized Stream Table



Ethylbenzene Production Facility Material Balance

Stream Number	1	2	3	4	5	6
Temperature (ºC)	25	25	19.7	25	25	437.6
Pressure (kPa)	110	2000	100	2000	2000	1990
Mass Flows (kg/hr)	7208.2	2994.7	15172.4	898.4	1048.1	16070.8
Molar Flows (kmol/hr)	90.65	106.21	195.74	31.86	37.17	227.61
ETHYLENE		98.78		29.63	34.57	29.63
ETHANE		7.43	0.64	2.23	2.60	2.87
PROPYLENE			5.95			5.95
BENZENE	81.58		180.07			180.07
TOLUENE	9.06		9.06			9.06
ETHYLBENZENE			1.34E-02			1.34E-02
1,4-DIETHYLBENZENE						

Stream Number	7	8	9	10	11	14
Temperature (ºC)	496.5	440	520.9	25	440	518.6
Pressure (kPa)	1988	1978	1975	2000	1965	1963
Mass Flows (kg/hr)	16070.8	17119.0	17119.0	1048.1	18167.1	18167.2
Molar Flows (kmol/hr)	205.55	242.72	209.64	37.17	246.81	212.24
ETHYLENE	-	34.57	1.47E-03	34.57	34.57	
ETHANE	2.87	5.47	5.47	2.60	8.08	8.08
PROPYLENE	13.53	13.53	15.01		15.01	15.02
BENZENE	165.59	165.59	133.99		133.99	99.42
TOLUENE	1.49	1.49	2.24E-03		2.24E-03	
ETHYLBENZENE	22.07	22.07	55.16		55.16	89.73
1,4 DIETHYLBENZENE			-		-	

Stream Number	15	16	17	19	24	25
Temperature (ºC)	13	11.3	15	142.9	11.3	15
Pressure (kPa)	100	110	100	120	110	100
Mass Flows (kg/hr)	679.1	17816.5	7964.3	9523.8	350.6	328.5
Molar Flows (kmol/hr)	17.44	202.78	105.09	89.71	9.46	7.98
ETHYLENE						
ETHANE	7.43	3.12	0.64		4.95	2.48
PROPYLENE	9.07	10.83	5.95		4.18	4.88
BENZENE	0.92	99.13	98.49	0.02	0.30	0.62
TOLUENE						
ETHYLBENZENE	2.23E-02	89.71	1.34E-02	89.69	2.23E-02	7.67E-06
1,4-DIETHYLBENZENE				**0 PPM**		
DEB Design Spec				**2 PPM**		