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OPTIMIZATION OF A FLUIDIZED BED REACTOR FOR THE PRODUCTION OF STYRENE FROM ETHYLBENZENE

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

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Approved by

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Abstract

In order to optimize Unit 500, a styrene production plant, the Net Present Value (NPV) was used as the objective function to ensure every optimization strategy had a positive economic effect. To optimize a chemical plant, it is important to note efficiency, economics, product specifications, and production requirements. The goal of this project was to make changes to the base case of Unit 500 to minimize the cost to produce styrene for an upstream unit. PRO/II was used to simulate various points in different unit operations throughout the process. The NPV was measured after each unit operation was simulated to compare economics between varying values. A proposed design has been made to increase the NPV and make a recommendation for moving forward. This report focuses on the optimization strategies for the styrene production facility and recommendations for continuing with this process.

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Introduction

This report focuses on the optimization of Unit 500, a styrene production plant. After simulating the base case, it can be seen that the process needed to be optimized to maximize the economics surrounding the process. A functioning kinetic process simulation was created using PRO/II, a steady state process simulator. From this process simulation, an economic model in Excel was updated to monitor the NPV after each unit operation change. Optimized values were justified based on having a positive effect on the NPV. Five or more data points were used for each major optimization step to ensure the optimum value was chosen. Topological and parametric changes were made throughout the optimization process. The base case was improved by 58%. The changes made to improve the base case are discussed throughout this report.

Safety Considerations

It is required that Styrene Production Plant, Unit 500, operates not only efficiently but primarily safely. All personnel are required to ensure that the plant operates in alignment with all Occupational Safety and Health Administrations (OSHA) guidelines and policies. Safe operation includes but is not limited to upholding standards pertaining to process safety, equipment safety, occupational safety. There are many risks associated with this process and factors that must be mitigated and addressed to remain within safe operating conditions. To fully address the various risks, it is recommended that a thorough Process Hazard Analysis is completed.

It is necessary to address chemical safety since there are hazardous materials present within this process. Some of these materials include ethylbenzene, styrene, benzene, toluene, methane, etc. OSHA requires that Safety Data Sheets (SDS) are provided to all personnel and individuals at risk of exposure for each hazardous chemical on site in order to communicate information concerning the hazards. Ethylbenzene, styrene, benzene, and toluene all have health and fire hazards. Additionally, styrene has reactive hazards, since it has the potential to self-polymerize at temperatures exceeding 125 degrees Celsius. The concentration of styrene increases in streams leaving the towers. In order to prevent a hazardous incident, it recommends that temperature controls are and alarm systems are installed to notify personnel when the temperature nears the temperature limit so a scenario resulting in equipment damage and/or exposure to personnel is eluded. Alarm systems should also be installed in other areas of the process to prevent exceeding pressure, level, flow, and temperature limits. This will notify personnel to adjust process conditions in order to reduce the possibility of a near-miss.

OSHA standards require that there is proper Personal Protective Equipment (PPE) selection and usage to remain in compliance. Due to the specifics of this process, it is applicable that personnel are knowledgeable about required PPE that may include but is not limited to hard hats, protective eyewear, fire retardant clothing, steel toe boots. The OSHA permissible exposure limit (PEL) for styrene and ethylbenzene is 100 ppm. Personnel should not be exposed to more than an average of 100 ppm styrene during a regular 8-hour workday, without respiratory protection. Respiratory protection should additionally be utilized in the event that inspections/ maintenance that require entering confined spaces and/or closed vessels with high concentrations of respiratory hazards are present; regular maintenance and inspections of facility equipment is required. Additional precautions should be taken to protect equipment integrity, such as PSVs for pressure protection as well as temperature controls, so metallurgy limits are not exceeded.

Environmental Considerations

All chemical production plants, including Unit 500, are required to operate within a certain operating range to ensure they meet all regulatory requirements set forth by the Environmental Protection Agency (EPA) and federal and state agencies. The Styrene Information and Research Center (SIRC) monitors the regulatory and policymaking activity on styrene and its production. In the United States, California and other states have different regulations; California has stricter regulations than the rest of the United States. The requirements set forth by various governmental agencies govern the manufacture, sale, transportation, use, and disposal of styrene. The EPA has deemed styrene as a chemical that is a hazardous air pollutant.

To ensure Unit 500 is operating within regulatory requirements, environmental considerations are a top priority. As styrene has been deemed a hazardous air pollutant, it is important to have minimum styrene escape into the atmosphere. Flare gas recovery systems can be included in the case of over pressurization to collect pollutants and recycle them back into our process. This would reduce pollutants in the atmosphere and minimize the escape of greenhouse gasses. Storage tank losses can be minimized by using double seals and vapor recovery systems. By having double seals, leaks are less likely to spill to the ground. This ensures maximum sealing safety. This prevents our materials from reaching the atmosphere and polluting the environment. A vapor recovery system will minimize emissions by reducing venting. While these considerations help minimize air pollutants, routine emissions monitoring should still take place to ensure the plant is operating within regulation and provide data to engineers and operators if the plant gets out of specification.

As engineers, it is our responsibility to ensure the styrene production plant is having minimal impact on the environment and surrounding ecosystems. One way to ensure this is to separate wastewater streams from the storm drainage system. Styrene is known to be carcinogenic to animals, so it should not escape into the storm drainage system, which would pollute the community and open bodies of water. A separate wastewater collection system needs to be in place, so chemicals do not end up polluting the surrounding community.

Global Cultural, Social, Environmental, and Economic Impact

Globally, styrene is used as a key material in manufacturing plastics, synthetic rubbers, and resin. These products are then used in various industries including electronics, automotive, and healthcare. Styrene is also a precursor to polystyrene. By the end of 2019, 15.61 million metric tons of styrene were produced. It is forecasted that the production of styrene will grow by 2024 to 15.68 million metric tons.

In the current state of the world, several current events have halted various industries and production. These events were unprecedented and had a severe impact on the economy. The production of styrene has not been exempt from these events. In December 2019, the world was struck by a pandemic commonly known as Covid-19. As styrene is commonly involved in the construction and automotive industry, less styrene was used during the shutdowns from the pandemic as production was halted. Prior to the impact of Covid-19, the chemical industry was predicted to have low to flat growth in all geographies besides Asia. There are inevitable long-term impacts, however, there is a slow-return to pre-Covid practices. In addition to the Covid-19 pandemic, Russia invaded Ukraine in early 2022. Ukraine exports approximately 1.9 billion pounds of ethylbenzene each year, which is a reactant in the production of styrene. This creates a shortage of ethylbenzene to make styrene. By having less styrene, the plastics industry finds itself in a shortage, with prices rising. With unforeseen circumstances such as political conflicts and pandemics, it is important to consider the global economic effect of the product created by Unit 500. With more styrene being created and fed to the upstream polystyrene unit, this could be helpful when shortages arise in various industries.

There are different regulations surrounding the production of styrene globally. The International Agency for Research on Cancer reviewed styrene most recently in 2018. In 2018, they deemed styrene to be in Group 2A, possibly carcinogenic to humans. This is not enforceable as regulation, however, it is often used as a reference in regulatory actions and policies. While countries such as China agree with this. Other countries such as Chile disagree and classify styrene as Group 4, probably not carcinogenic to humans. The European Union has no regulation of carcinogens, reproductive toxinogens, or occupational exposure limits. However, many countries have implemented limits on styrene food contact exposure. The United States and Japan have air emissions standards for styrene pollutants, but this is not regulated in every country.

Styrene is important to the global industry. It is widely used and enables many products to generate cost-effective benefits. Styrene strengthens military equipment, cushions bicycle helmets, and helps create wind powered turbines. The uses of styrene are endless. The production of styrene not only assists industry, but also contributes to the reduction of greenhouse gas emissions by providing energy efficient insulation. The production of styrene and use of styrene will continuously increase as it is energy efficient and reduces the global dependency on costly natural resources such as tropical woods, marble, and granite.

Base Case Overview

Unit 500 is a styrene production plant that is intended to supply styrene to an upstream unit for the production of polystyrene. The proposed design is for a grassroots facility that would produce 100,000 tonnes per year for twelve years after start-up. This plant is predicted to take two years to construct and will begin production on January 1, 2024.

Process Description

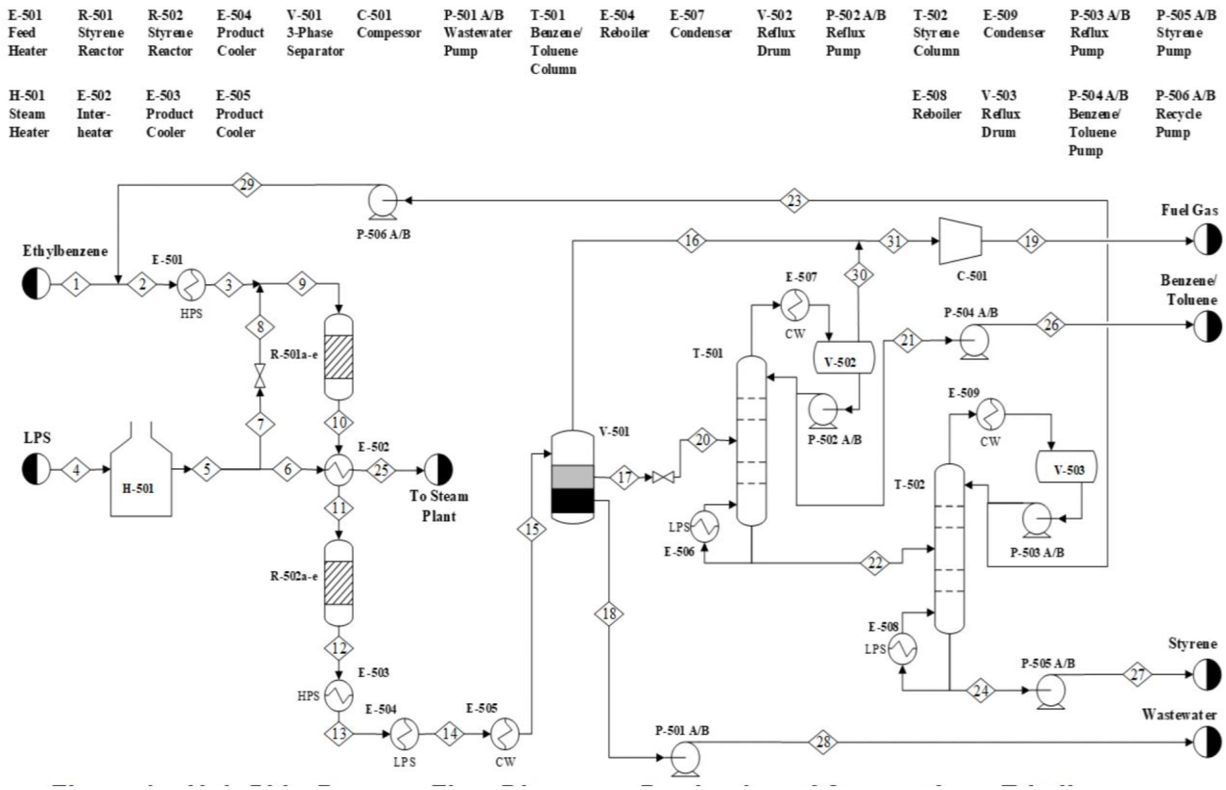
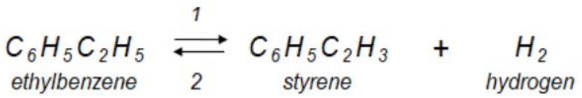


Figure 1: Process Flow Diagram for the Base Case of Unit 500

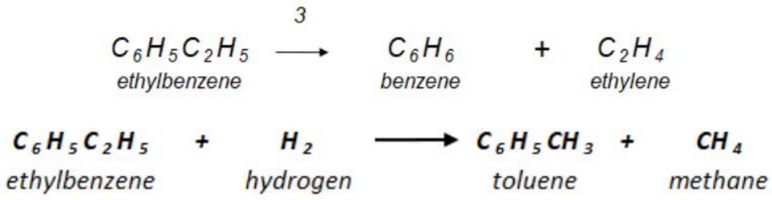
Unit 500 must produce 100,000 tonnes per year of styrene (120 kmol/hr) while operating for 8000 hours per year and meeting a product purity specification of 99.8 wt% styrene. These are required specifications and may not be altered for optimization purposes.

Liquid ethylbenzene, alongside benzene and toluene is combined with recycled contents in to form a stream containing the previously mentioned components and styrene. This is then sent directly to the first heat exchanger in the process, E-501. Within the heat exchanger, the process stream is heated through the use of high-pressure steam. The resulting vapor product stream, then mixed with Stream 8 to form Stream 9. Simultaneously, low-pressure steam, Stream 4, enters a heater exits as Stream 5. The steam in Stream 5 then splits into Stream 6 and Stream 7. Stream 9, now consisting of all vapor components in both Stream 3 and Stream 8, enters the first set of reactors, styrene reactor, R-501a-e. All styrene production reactions take place in this reactor. These reactions include the dehydrogenation of ethylbenzene to produce both styrene and hydrogen:



$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \underset{2}{\overset{1}{\rightleftarrows}} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2}$$

and side reactions to produce both benzene and toluene:



$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \xrightarrow{3} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \longrightarrow \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4}$$

The reactor effluent, Stream 10, enters the second heat exchanger E-502. The low-pressure steam in Stream 6 enters heat exchanger E-502 and heats the process stream, Stream 10. The components of Stream 11 exit the heat exchanger and enter into the second set of styrene reactors R-502a-e. Reactions identical to those previously mentioned take place in reactors R-502a-e in order to reach a higher conversion of styrene. Upon accomplishing this, the second reactor's effluent exits in Stream 12.

Streams 13-20, V-501, C-501 Section

The reactor effluent temperature is cooled further as Stream 13 passes through E-504. Stream 14 takes the vapor stream through another heat exchanger, E-505. This vessel is a three-phase separator, flashing at feed conditions. The purpose of this vessel is to remove the bulk of the methane, leaving in Stream 16 as a vaporous mixture, and remove the bulk of the water, leaving in Stream 18 as liquid. The organic liquid phase is sent from V-501 through stream 17 to a regulator valve, to adjust the pressure and temperature before distillation. Stream 16 is mixed with another vaporous stream containing methane, Stream 30, to form Stream 31 which is to pass through C-501. Stream 19 is the exiting stream of the compressor, containing fuel gas product.

T-501 Section

The organic liquid phase from the 3-phase separator is then sent to the first column, T-501. This column is where benzene and toluene are separated out of the organic liquid stream. The light key which is primarily composed of benzene and toluene and additional lighter components rise up the tower and into the distillate stream. The distillate stream, which is in vapor phase, is sent to E-507, the overhead condenser, where the stream is cooled utilizing a utility stream of cooling water. The cooling water stream temperature range is from 30 C to 45 C. The condensed liquid stream is sent to V-502, the reflux drum, where a liquid level is constantly held. Following this, the reflux pump, P-502A/B, cycles the liquid back to the top of the tower to provide cooling and condensation of the vapors present. The remainder of the condensed liquid stream is pumped through P-504 A/B as a Benzene/Toluene product stream. The overhead product specifications include 99% purity Benzene and Toluene in order to reach prime separation efficiency in the tower. At the bottom of the tower, an organic liquid stream composed of heavy and light components are split and sent through a reboiler where the organic stream is vaporized utilizing the LPS utility stream. This stream is cycled back through the tower, while the remainder of the stream exits the tower as bottoms product. The bottoms product exits the tower; it is primarily composed of the heavy key Ethylbenzene and Styrene.

T-502 Section

Products leaving the bottoms of tower T-501 are fed directly into T-502 where further distillation will occur. This second distillation column acts to separate styrene from other components. The bottoms of the tower will produce the 99.8 weight % styrene that is to be sold. The bottoms product is split so that some of the stream goes to the reboiler E-508, and the rest is sold at a rate of 100,000 tons/year. The distillate of T-502 will be used as a recycle for the entire process. The distillate enters a condenser, which prepares the stream to enter vessel V-503. V-503 liquifies the stream and provides the reflux back to the column. The liquid stream leaving the vessel is sent to pump P- 503 then split to send part of the stream back to the column and the rest to the recycle stream.

Sensitivity Analysis

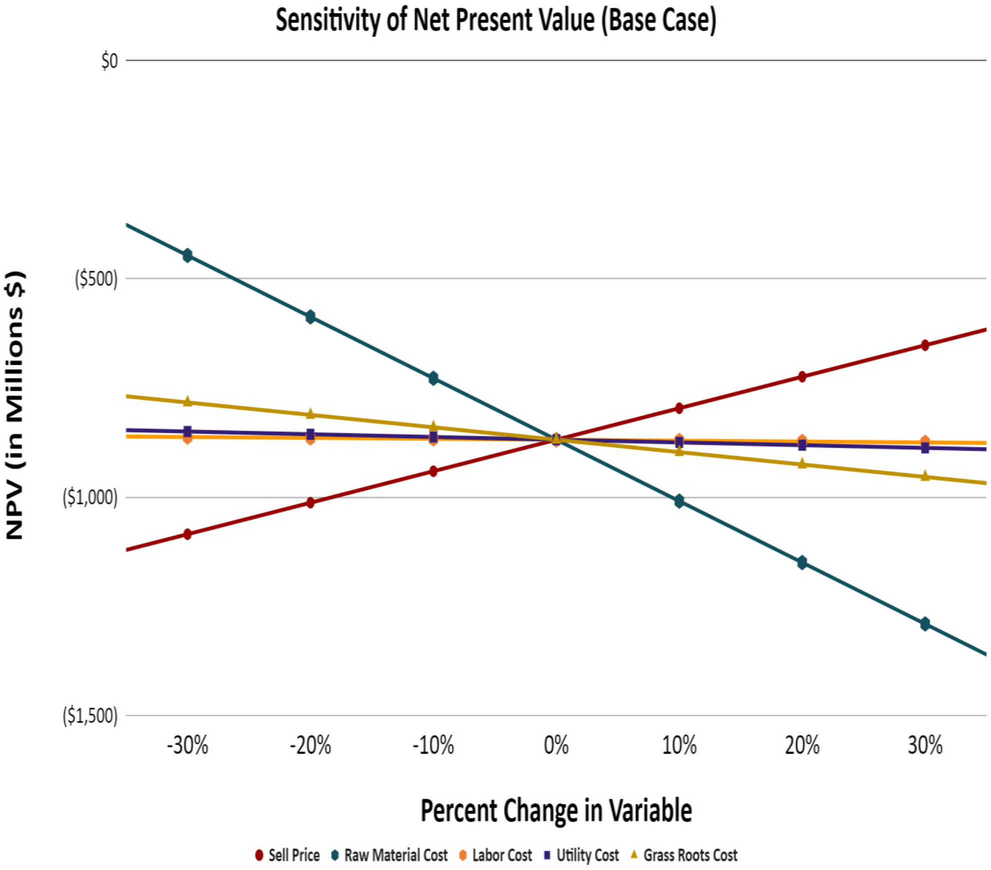


Figure 2: Sensitivity Analysis of the Base Case of Unit 500

The figure above shows the sensitivity graph, which shows how sensitive the NPV is to a set of variables. The two variables that affect the NPV the most are the sell price of styrene (the red line) and the raw material cost (the navy blue line). Since ethylbenzene is the only raw material, this variable is effectively the purchase price of styrene. Because the styrene production unit is not a standalone unit but rather one in a series, the prices of ethylbenzene and styrene are transfer prices between two units. Since styrene is being sold to a downstream unit within the company, and potentially bought from another unit within the company, the purchasing and selling prices are not the most accurate variable to describe how these change the net present value. Instead, a more accurate and useful way to interpret these two variables is to view the combination of them as how well ethylbenzene can be utilized; that is, how efficient is our process at converting all the purchased ethylbenzene into styrene.

For the reaction portion of the process, the goal is to convert a maximum amount of ethylbenzene to styrene to ensure a high yield and selectivity of reactions. This ensures all the side reactions and production of undesirables is kept to a minimum, and ethylbenzene is effectively being converted to styrene. For the separation portion of the process, this means that preventing losses of either ethylbenzene that could be recycled, or styrene that should be sent to the product stream.

Importance of Optimization

Unit 500 is a proposed unit that would send its styrene product to a downstream polystyrene production facility. Because of this, styrene is a necessity. The two main options become whether to purchase styrene, or to produce it within the company. After simulating the base case economic model, purchasing styrene was cheaper than making styrene. Thus, optimization becomes a necessary step in order to make an informative decision of whether to purchase or manufacture styrene. The goal of the optimization is to maximize the NPV of the project, and once the NPV has reached its maximum, to come to a conclusion about whether to proceed with the production of Unit 500.

Optimization Strategies

Reactor Optimization

The main optimization goal was to increase the selectivity and yield of styrene. To optimize the adiabatic packed bed reactor, multiple variables were manipulated in order to make parametric changes to the process. In contrast, the reactor material of construction, which is stainless steel, solid catalyst bed volume and the reactor volume, which are 50 m^3 and 83.3 m^3 respectively, remained constant. The variables that were considered for optimization included the reactor temperature, pressure, L/D ratio, and steam dilution. Although changing the reactor pressure was considered, it was not implemented in the optimization cycle. This is mainly due to the minimal NPV changes that were detected as a result of increasing and decreasing the reactor feed pressure. The pressure within the reactor is in an acceptable range to ensure that the materials within the reactor remain in gas-phase. Since the reaction does occur in gas-phase, operating at a pressure between 1 and 10 bar does not have a significant effect on the selectivity or overall cost of the process. Thus, it was determined that it was more beneficial to proceed with primarily optimizing reactor temperature, L/D ratio, and steam dilution. As a result of all the reactor optimization strategies, there was an overall increase of approximately $70.8 M. Additionally, there was a 27% increase in selectivity and a 10% increase in yield. Although there was a decrease in conversion, the ethylbenzene that is not converted to the desired product will be recycled without making significantly harsh impacts on the NPV due to implemented optimization tactics.

Temperature

To optimize the reactor temperature, the reactor temperature was decreased in R-501 and R-502 by 2% and 6% respectively. Utilizing AVEVA Pro/ll Simulator, temperature cases above and below the base case temperatures were studied to view their effect on the economic model for the process. In order to simulate this within Pro/ll, the process stream temperature entering the reactors was specified using the heat exchangers prior to the reactor inlet. The decrease in temperature within the reactor allowed an increase in the selectivity of styrene. This is because there are multiple reactions that take place within the reactors, and the reaction that produces styrene takes place at a relatively lower activation energy than the reactions that produce the undesired products such as benzene and toluene. For example, the styrene producing reaction occurs at an activation energy of 90,981 J/mol whereas the benzene producing reaction occurs at an activation energy of 207,989 J/mol. In technical applications, reactions with lower activation energies react more efficiently at lower temperatures. As a result of decreasing the temperature in R-501, there was a $4.5 M increase in NPV. There was an additional increase of $20 M in NPV as a result of decreasing the temperature in R-502. There was likely a larger change in NPV in R-502 due to the reaction kinetics and the resultant reactant to product ratio leaving R-501. Prior to entering reactors, the process stream is diluted with steam. In finalization of this process production a temperature control should be implemented to ensure drastic variations in the reactor temperature do not occur. Below are figures that illustrate the changes in NPV due to changes in the reactor temperature. In the figures, the red point represents the optimized case while the green point represents the base case.

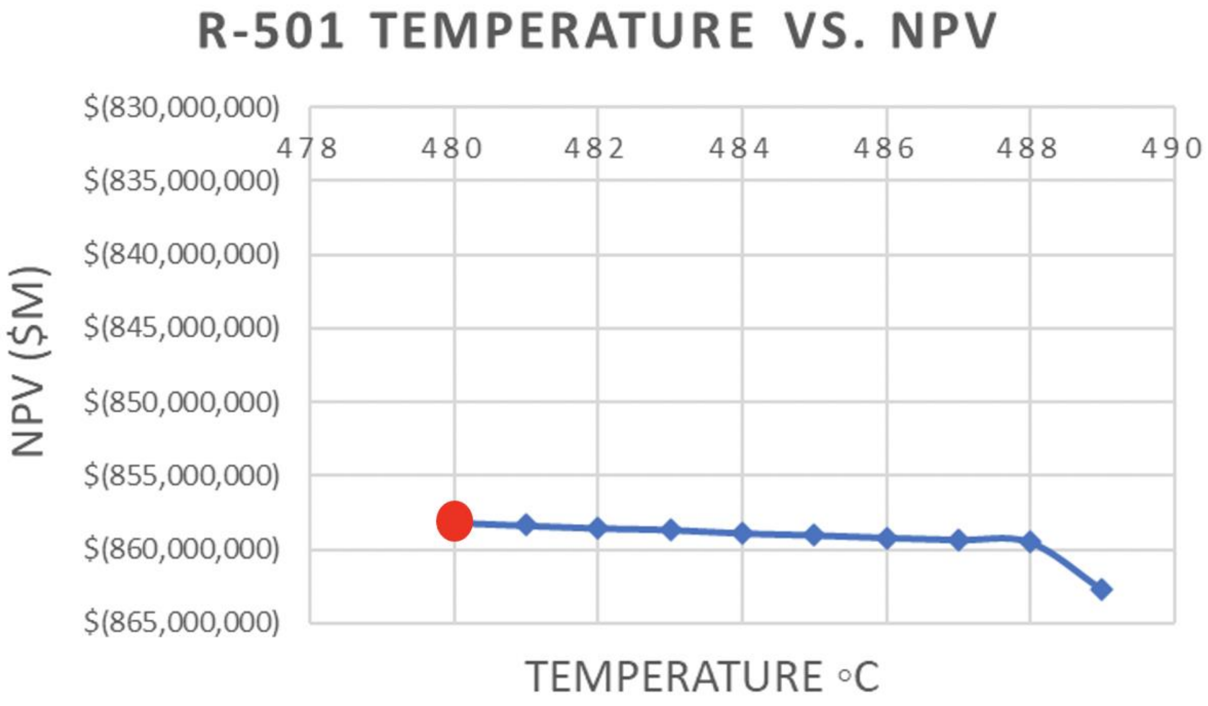


Figure 3: R-501 Temperature vs NPV

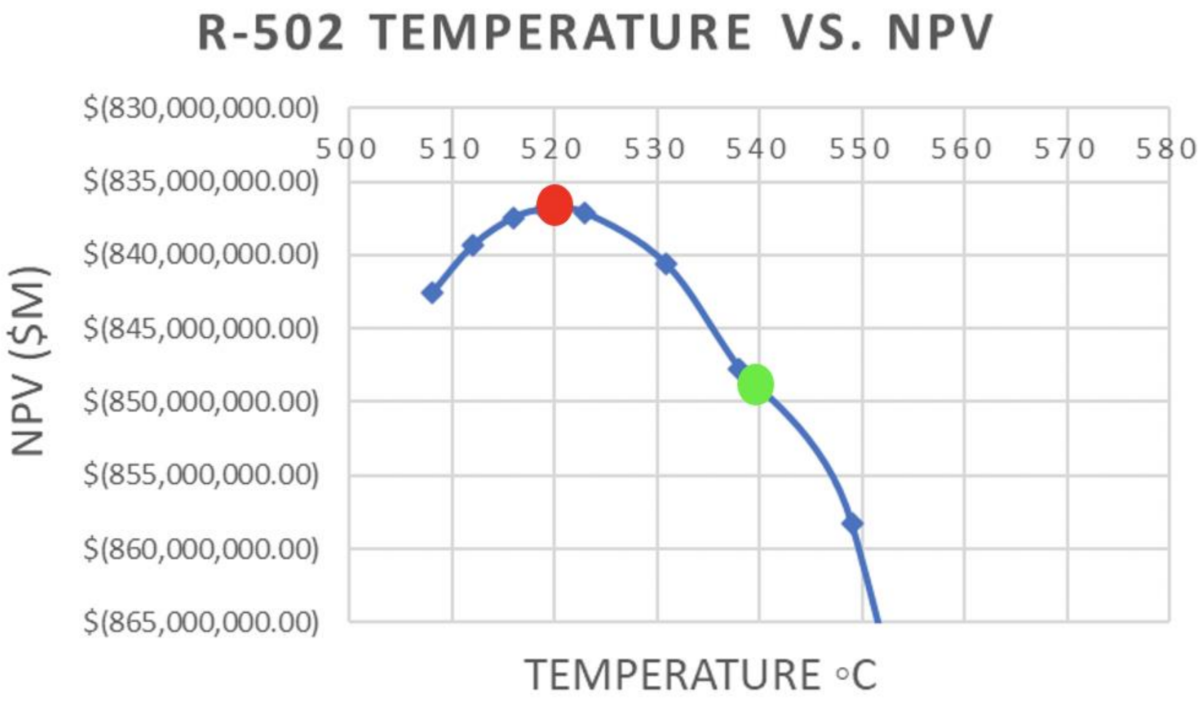


Figure 4: R-502 Temperature vs NPV

Length to Diameter (L/D) Ratio

To optimize the reactor, the L/D ratio entering both R-501 and R-502 was decreased from the base case of 3 to 2.5. The L/D ratios were considered to be limited to an optimum range of 2-10. Heuristic data suggest that in most processes the L/D ratio is optimum between 2-5 (3). In order to alter the L/D ratio the reactor volume was kept constant at 83.3 m^3 as previously mentioned while the length and the diameter of the reactor were changed. The base case L/D ratio yielded a length of 9.84 m and a diameter of 3.28 m. As a result of decreasing the L/D ratio the length decreased to 7.51 m whereas the diameter increased to 3.76 m. The proper length and diameters that corresponded to each L/D ratio for the specified reactor volume was calculated using Excel. The logic that technically supports decreasing the L/D is heavily based on the effect L/D ratio has on pressure drop. Pressure drop increases along the length of a reactor. Since a smaller L/D ratio results in a decrease in the length of the reactor while achieving the same reactor volume, it leads to a decrease in pressure drop. A decrease in pressure drop leads to an increase in reactor fluid outlet pressure. As a result, the process stream is at a higher pressure entering V-501, the three-phase separator. A higher pressure in this vessel leads to an increase in vapor density which minimizes the loss of ethylbenzene to the fuel gas stream. As a result of this optimization tactic, there was a $46 M increase in NPV.

Steam Dilution

Within the process, incoming LPS is heated within H-501 and combined with reactor feed as a diluent. By diluting the reactor feed there was a decrease in the concentration of ethylbenzene as well as other reactor constituents. Ethylbenzene is also required for the undesired reactions to occur as well. By increasing steam dilution, the selectivity of styrene is increased and is favored rather than the undesired by-products such as benzene and toluene, due to the reaction kinetics and the reaction order of the undesired reactions. The base case steam flow was specified as 3900 kmol/hr and was increased to 4500 kmol/hr in the optimized case by varying the splitter specification leaving H-501 in Pro/ll. As a result of increasing the steam dilution flow, there was a $288 K increase in the NPV.

Separations Preparations

To improve the separations preparations, the temperature entering the three-phase separator, V-501, was decreased. The temperature was decreased to improve the efficiency of the separations by minimizing the loss of ethylbenzene to the fuel gas stream. Cooling water was used to lower the temperature from 65 degrees Celsius to 40 degrees Celsius. The cooling water was adjusted by changed the specification of the utility stream from E-505, a simple heat exchanger. By decreasing the temperature, the percent of ethylbenzene recovery increased from 97% to approximately 99.9%. As a result of decreasing the temperature, there was a $77 M increase in the NPV. This is shown in the figure below. While it can be seen that the optimum temperature is below 40 degrees Celsius, the temperature can not be below 40 degrees Celsius using cooling water as the utility stream. Refrigerated water can be explored as an alternative utility, however, this could increase the required duty which would increase the cost of utilities.

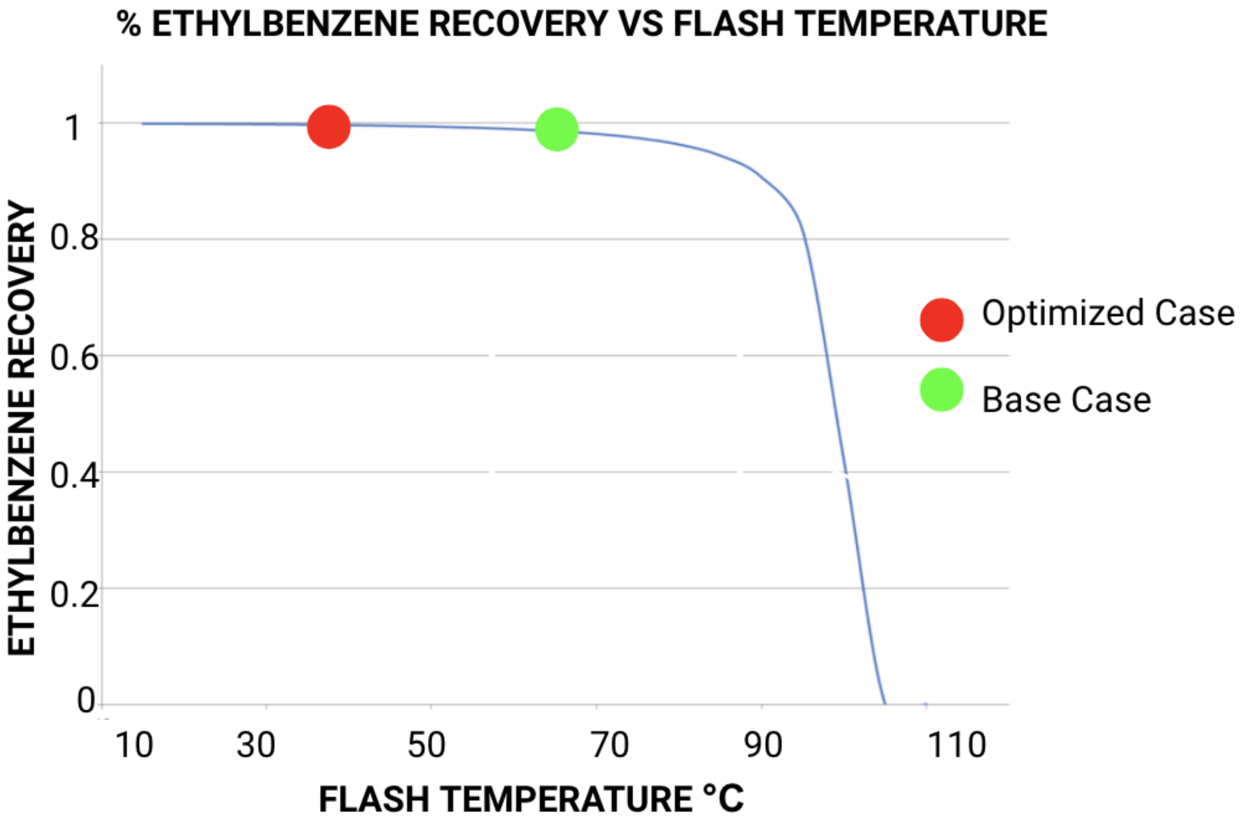


Figure 5: Percent Ethylbenzene Recovery vs Flash Temperature in V-501

Separations

T-501 Conditions

The top tray pressure of T-501 was increased to reduce the volumetric flow of the vapor to increase the concentration of styrene in the bottoms going into T-502. The increase in top tray pressure will permit a higher reflux rate, so more undesired products will exit in the vapor stream. This increases the efficiency of the separations, as styrene is the desired product. To increase the top tray pressure, the valve allowance before T-501 had to be increased to increase the inlet pressure. The inlet pressure was increased by 10 kPa from the base case (60 kPa in the base case and 70 kPa in the optimized case) and allowed the top tray pressure to be increased by 10 kPa as well. The base case top tray pressure was 40 kPa, while the optimized top tray pressure was 50 kPa. This allowed for a NPV increase of $6 M.

T-501 Materials of Construction

In the base case of Unit 500, the towers, T-501 and T-502, were constructed out of Titanium. In the optimization of Unit 500, Carbon Steel is being used as the material of construction for the towers. Carbon Steel is more cost-effective and is rated for the process conditions and materials. Styrene is rated C-Fair for its compatibility with Carbon Steel, while ethylbenzene, toluene, and benzene are all rated A-Excellent.
By using Carbon Steel instead of Titanium, the NPV has a positive increase of $131 M. This had the largest impact on the NPV.

Compressor

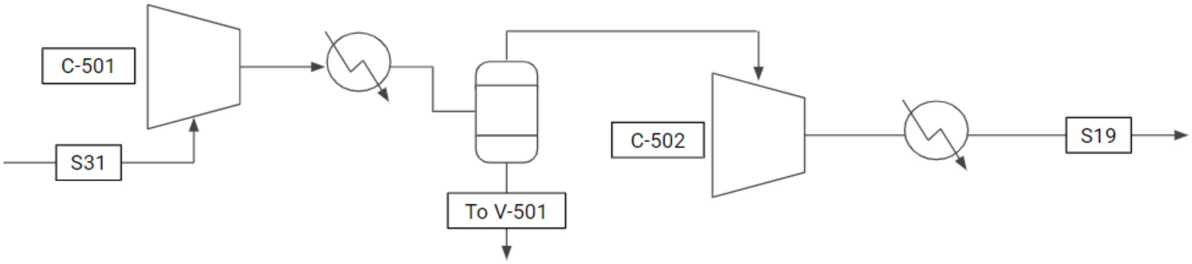


Figure 6: Proposed topological changes to C-501

After the fuel gas leaves the top of the 3 phase separator, it is then sent to a compressor before being sent off as the product stream. In the base case, this is only one large compressor with a compression ratio of 6:1. This needed to be changed because of both safety and economic considerations. The first economic consideration was to add another compressor in series, or multistage compression. Heuristic data suggest that for efficiency purposes, a compressor should operate in a compression ratio range from 2-4 (3). Similarly, all compressors in series should have the same compression ratio, as this minimizes the overall amount of power used by each compressor. In the optimized case, the minimum number of compressors to have the stage compression ratio fall in the suggested range was 2. In the optimized case, both compressors operate at a compression ratio of about 2.5.

For both economic and safety considerations, an intercooler was introduced in between the compressors. This intercooler, coming immediately after the first compressor, lowers the temperature of the gas before being sent to the next compressor. This serves two purposes; first, lowering the temperature of the gas allows the second compressor to run more efficiently and use less power, and secondly, cooling the gas stream allows any moisture that was in the gas to condense out of the vapor stream before going into the compressor. In order to catch any condensate, a knockout drum would be needed, whereby any potential liquid in the drum would be recycled to the 3 phase separator. The final safety consideration is the exiting temperature of the fuel gas leaving the second compressor. Heuristic data suggest that the fuel gas stream should be no hotter than a range of 170-200 degrees Celsius (3). This aftercooler on the second compressor is a safety precaution that ensures that the gas doesn't exceed the average of this range.

Purchase vs Produce

With the NPV maximized via the optimization strategies discussed above, there is now the choice of whether to purchase or to produce styrene. The market price of styrene is $1,598/MT (3), and the equivalent market price of the optimized case is $2,288/MT. Thus, purchasing styrene is cheaper than manufacturing it. However, a recommendation should be based on more than just the numbers. Although manufacturing styrene is more expensive than purchasing it, there are a number of advantages to consider. Firstly, by manufacturing styrene, the styrene source is less susceptible to shortages or procurement/delivery issues from vendors. Also, by manufacturing styrene, the location of the plant is decided by the company. If styrene were to be purchased, there is no control over where the styrene was physically coming from, and this could introduce increased transportation costs, as well as aforementioned procurement issues. Finally, there would be no way to ensure the quality of styrene. Styrene needed for the polystyrene unit should be 99.8% pure by weight and purchasing this from a vendor means that there would be no way to ensure this.

While the optimization presented does not include a proper risk analysis to determine the value of being able to mitigate these concerns, from the perspective of the engineers that oversee production units such as this, the value of having this control over the process cannot be overstated. Having control over the procurement and quality of the resources needed for the polystyrene unit would serve to prevent inefficiencies and downtimes that could compound and magnify in downstream production.

Additional Optimization Strategies

Hybrid Feed Source

As an additional optimization strategy, it is recommended that alternative ethylbenzene feed sources are considered.It is possible to implement a hybrid feed source of ethylbenzene. The base case economic model with an NPV of - $862M was developed based on the proposition that all the ethylbenzene feed would be supplied by the on-site ethylbenzene production unit. The current transfer price is at $1,268/MT

(3). Based on an economic analysis of current market data, the purchase of ethylbenzene is available for as low as $600/MT (1). While outsourcing an optimum ratio of ethylbenzene feed, the onsite production unit could still be utilized to fulfill the remaining Unit 500 needs. While conducting the alternate ethylbenzene feed source process, the feed unit could choose to sell the excess product to prospective clients or make less product. This option provides the opportunity to nearly increase our NPV by 40% with $100-$200 M gains in NPV. As seen in the sensitivity table, the cost of raw materials has a large impact on the current economics of the styrene production process. Another option that can be considered in order to reduce the raw materials costs is to discuss the proposal of lowering the transfer price of ethylbenzene in order to ensure it more accurately reflects the current market price of the material and aids in the optimization of plant profitability.

Addition of Refrigerated Water

As discussed previously in the text, more ethylbenzene is recovered in V-501 if the temperature is lowered. However, the minimum temperature in V-501 is limited by the cooling water in the heat exchanger prior to the vessel. The coldest the process stream can get entering the vessel is 40 degrees Celsius, as this is the lowest the cooling water temperature can get the process stream without violating a minimum approach temperature of 10 degrees Celsius within the heat exchanger. In order to further cool the stream, another heat exchanger would be added after the cooling water heat exchanger, but instead would contain refrigerated water, which could get the process stream as cold as 10 degrees C.

As noted by the Ethylbenzene Recovery vs. Flash Temperature graph, the colder the vessel is, the more ethylbenzene is recovered. This recovery of ethylbenzene faces diminishing returns as the temperature is decreased, and there comes a point at which the added cost of refrigerated water to lower the temperature is not worth the recovery of ethylbenzene

Introduction of Fluidized Bed Reactor

Fluidized bed reactors have long been used in industry as a means to carry out necessary reactions for the production of chemicals. They are harder to design, construct, and operate than other types of reactors commonly used in industry (4). The purpose of introducing a fluidized bed reactor in this analysis is to explore an alternative reactor type for the production of styrene from ethylbenzene, while still remaining both economically and safely optimal.

For the introduction of a fluidized bed reactor, a number of design constraints were outlined: an inlet feed pressure ranging from 0.75 to 5 bar, an inlet feed and reactor temperature ranging from 300 to 750 degrees C, the reactor volume, an L/D ratio ranging from 2 to 10, and a minimum conversion of 5%. Note that of these constraints, the only constraint that was chosen during the optimization of the reactor was the choice to set the minimum conversion to 5%. Theoretically, there is no constraint for the conversion of a reactor, but as outlined by previous sections, the economic limitation is rooted in how expensive the reactor operates when integrated into a plant. For this specific set of reactions, the yield of reaction increases when the conversion of styrene decreases. From a fundamental standpoint as outlined by the sensitivity table, a higher yield (and thus lower conversion) is necessary. While it is true that at conversions that are lower than 5%, the reactor alone could operate at more economically viable conditions, a high recycle would be required in order to retain the production goal. For the reactor, this is not an issue, but further downstream in a process, a higher recycle necessitates a larger tower/separation unit. This means that the reactor operates at an economic optimum when the increase in yield (and lowering conversion) is not offset by a higher equipment and utility cost for separations due to the consequent lowered yield. To determine this “tipping point,” a much more rigorous analysis is required, but for the purposes of this investigation, a minimum conversion of 5% was chosen based on past experience.

The fluidized bed reactor was simulated using Aveva’s PRO II process simulator. Because the simulator does not have the capability to simulate a fluidized bed, the bed was closely approximated using a packed bed reactor with a bypass to simulate the channeling that could occur in a fluidized catalyst bed. As outlined in the section above, the inlet parameters were changed, and the objective function for this optimization was the yield and selectivity of reaction. As previously discussed, the yield and selectivity is not a wholistic view of an economic optimum for a reactor, but when analyzing the reactor alone, it is an appropriate metric to follow. PRO II has the capability to optimize a variable given a set of input variables to change and a number of constraints. This optimizer uses linear optimization, which is akin to the process of taking one input variable at a time while holding all other variables constant, finding an optimum yield, and then repeating the process with the next variable until a maximum across all variables has been reached. It is important to note one short coming of this method; given that the output variable is a multivariable function, the global maximum of the range is not necessarily at the combination where all the input variables showed a maximum output individually, while all other variables are held constant. However, there is sound basis in this approach, and for these purposes, it was appropriate.

The maximum selectivity calculated for this reactor was approximately 11.8 at a conversion of 5% (the minimum). This selectivity is acceptable and means that for about every 12 parts of styrene produced (by mole), there is 1 part of undesired products produced. One additional constraint worth noting is that for the fluidized bed reactor to operate properly, the minimum fluidization velocity must be met. This is to ensure proper fluidization of catalyst particles to properly manipulate the reaction kinetics. However, the gas velocity must not be too high, or else catalyst erosion, a phenomenon in which the catalyst acts as an abrasive to the reactor wall, or blowout, which is literally blowing the catalyst out of the reactor, could occur. For this simulation, the gas velocity is approximately 3.83 times the minimum fluidization velocity, which falls into an acceptable range.

For this study, the reactor was not priced, but note that this reactor is essentially one large tube (as opposed to multiple) with heating tubes going into the reactor in order to operate isothermally. Thus, the reactor will also have a utility cost associated with it.

Conclusion

It is recommended that the production of the styrene unit be continued, with the additional recommendation that a proper risk analysis be conducted to accurately determine the value of controlling the procurement and quality of styrene being sent to the downstream polystyrene unit. Note that “moving forward” does not mean moving to construct the facility, but rather to continue to a more rigorous analysis of this facility.

Appendix A: Stream Tables

Note that the stream tables in this report have values that have been rounded for the sake of readability. A more detailed version of this stream table can be found in the Excel file accompanying this report

Stream No.	1	2	3	4	5	6	7	8	9	10	11	12
Temperature (℃)	136	100	225	159	800	800	800	799	510	487	490	482
Pressure (kPa)	222	222	202	600	565	565	565	200	230	188	173	145
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)	22164	143124	143124	147725	147725	66657	81069	81069	224188	224188	224188	224188
Total Flow (kmol/h)	210	1349	1349	8200	8200	3700	4500	4500	5849	5959	5959	6005
Component Flows												
Water	0	0	0	8200	8200	3700	4500	4500	4500	4500	4500	4500
Ethylbenzene	205	1343	1343	0	0	0	0	0	1343	1215	1215	1153
Styrene	0.00	1.48	1.48	0.00	0.00	0.00	0.00	0.00	1.48	105	105	149
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	85	85	113
Benzene	2.10	2.10	2.10	0.00	0.00	0.00	0.00	0.00	2.10	8	8	11
Toluene	2.10	2.46	2.46	0.00	0.00	0.00	0.00	0.00	2.46	21	21	37
Ethylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6	6	9
Methane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	18	18	35

Stream No.	13	14	16	15	17	18	19	20	21	22	23	24
Temperature (℃)	270	180	35	35	35	35	277	35	52	124	91	124
Pressure (kPa)	130	115	100	100	100	100	240	70	50	70	25	55
Vapor Mole Fraction	1	1	1	0	0	0	1	0	0	0	0	0
Total Flow (kg/h)	224188	224188	1557	224188	141914	80717	2174	141914	5009	136274	120959	15315
Total Flow (kmol/h)	6005	6005	167	6005	1358	4480	183	1358	54	1286	1139	147
Component Flows												
Water	4500	4500	9	4500	11	4480	19	11	1	0	0	0
Ethylbenzene	1153	1153	3	1153	1149	0	4	1149	11	1138	1138	0
Styrene	149	149	0	149	148	0.00	0	148	0	148	1	147
Hydrogen	113	113	112	113	0	0.00	113	0	0	0.00	0.00	0.00
Benzene	11	11	0.24	11	10	0.00	2	10	9	0.00	0.00	0.00
Toluene	37	37	0.29	37	37	0.01	3	37	34	0.37	0.37	0.00
Ethylene	9	9	8	9	1	0.00	9	1	0	0.00	0.00	0.00
Methane	35	35	33	35	1	0.03	35	1	0	0.00	0.00	0.00

Stream No.	25	26	27	28	29	30	31
Temperature (℃)	791	52	121	35	93	50	37
Pressure (kPa)	550	200	200	200	222	50	40
Vapor Mole Fraction	1	0	0	0	0	1	1
Total Flow (kg/h)	66,657	5,009	15,315	80,731	120,959	617	2,174
Total Flow (kmol/h)	3,700	54	147	4,481	1,139	16	183
Component Flows							
Water	3,700	1	0	4,481	0	9	19
Ethylbenzene	0.00	11.17	0.29	0.05	1,138	0.32	3.51
Styrene	0.00	0.16	147	0.00	1.48	0.00	0.27
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.32	113
Benzene	0.00	8.58	0.00	0.00	0.00	1.81	2.05
Toluene	0.00	34	0.00	0.01	0.37	2.50	2.79
Ethylene	0.00	0.02	0.00	0.00	0.00	0.86	8.52
Methane	0.00	0.01	0.00	0.03	0.00	1.26	35

Appendix B: Equipment Tables

Plug Name		R-501A-E	R-502A-E
Plug Description			
Temperature	C	482.4704	482.1078
Pressure	KPA	139.2785	65.877
Number of Tubes		5	5
Reactor Length	m	10.91	8.72
Tube Inside Diameter	m	3.117	3.486

Hx Name		H-501	E-501	E-502	E-503	E-504	E-505	E-510	E-511
Hx Description									
Duty	M*KJ/HR	291.62	58.88	30.32	107.51	32.61	281.55	0.42	0.66
LMTD	C	n/a	n/a	233.46	n/a	n/a	64.52	78.04	90.53

Compressor Name		C-501	C-502
Compressor Description			
Pressure	KPA	96	240
Temperature	C	144.37	214.42
Actual Head	M	32116.41	39363.71
Shaft Work	KW	222.21	272.36
Isentropic coef., k		1.28	1.26

Column Name		T-501	T-502
Column Description			
Condenser Duty	M*KJ/HR	-91.3	-416.1
Reboiler Duty	M*KJ/HR	121.7	406.0

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(4) Cocco, Ray, et al. “Introduction to Fluidization.” *Back to Basics*, AIChE, Nov. 2014.