

OPTIMIZATION AND COST COMPARISON OF REACTOR TYPES
IN A STYRENE PRODUCTION PROCESS

by
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Dedication

To Gordon and Jo Cozadd, my Gampy and Diggy,
for instilling in me a love of learning from a very young age
and for being my best friends.

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There are several people without whom this thesis would not have been possible.

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Abstract

The focus of this thesis is to use the equivalent annual operating costs of isothermal, adiabatic, and packed bed reactors in order to determine which reactor is most cost effective in a styrene production process. In order to understand the steps leading up to this comparison, background information is first given regarding chemical engineering design, optimization, and process simulation. This information was necessary for completing the ChE 451 design project, which was to analyze the base case styrene process before optimizing it, in fall 2018. The results of this project are briefly outlined in the second section. The third section discusses fluidized bed reactors and the process which must be taken to model it in Excel. In this project, the selected configuration is three fluidized bed reactors, each with a volume of approximately 83 m^3 , in parallel. The last section discusses the calculation of equivalent annual operating costs for the isothermal, adiabatic, and fluidized bed reactors. Overall, fluidized bed reactors are found to be the most cost effective in the styrene process based on the equivalent annual operating costs; however, a comparison based on the net present value of the entire styrene process containing each reactor would yield a more accurate comparison.

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Chapter 1: Introduction

I. Introduction to Chemical Engineering Design

In their careers both as students and as professionals in industry, chemical engineers will likely be required to complete process design. Process design starts with defining a customer need and then developing profitable solutions to fulfill it. For chemical engineers, design projects focus on chemical processes and plants. In industry, one can expect to encounter three types of projects: modification to existing plants, scaling to a new production capacity, and design of a new process. The first makes up 50% of all projects, the second 45%, and the last only 5%.

Ultimately, the design process can be seen as the culmination of the entire chemical engineering field. It requires the engineer to demonstrate an understanding of mass and energy balances, separations and reactor unit principles, equipment sizing heuristics, and economic terms and calculations. However, the engineer must also take into account the constraints on the process due to the physical properties of its components, the local, state, and federal government regulations, the properties of the equipment materials, and the economics. To determine the best design for a specific process, the design process will be completed iteratively.

The design process has seven steps that fit into two phases: process design and plant design. Process design begins with identifying the design objective. The design basis is then set, and this takes into account the desired production rate and purity, the system of units, the design codes, the raw materials, and the utilities. Next, potential design concepts are generated, and these undergo analysis and evaluation in computer

simulations before one is ultimately selected. Plant design begins with creating a detailed equipment design. Then, it undergoes procurement and construction before it begins operation.

II. Introduction to Optimization

Although designing a new process is the least encountered project in the workplace, it remains important for the chemical engineer to know how to navigate the design process for a new plant. In addition to testing the engineer's overall knowledge of the field, it tests whether one really understands how to utilize optimization. This plays a key role in the analysis and evaluation of the potential design concepts for a process, and it can determine whether the overall project will even be fit for implementation.

According to Richard Turton's "Analysis, Synthesis, and Design of Chemical Processes," optimization "is the process of improving an existing situation, device, or system such as a chemical process." The goal of optimization is to find the best possible setup for the chemical process. Engineers work toward this best setup by changing specifications from a preliminary process design called a base case. Certain aspects of the process, such as its primary product and the sections of the plant, will not change during the optimization process. Therefore, an engineer must analyze the process to find potential improvements in operating conditions. These are called design variables, and they can be categorized as either continuous or discrete. Continuous variables, such as the temperatures and pressures in towers and reactors, can take any value within specified boundaries, or constraints. Discrete variables, such as the number of trays in a tower, must have integer values.

In order to quantify the degree of improvement resulting from a change in the process, there must be a defined point of comparison directly affected by the values of the decision variables. In the optimization process, this is called the objective function. If the objective function is a cost, it must be minimized during optimization; likewise, if it is a profit, it must be maximized. Ultimately, there are two different types of optimums that can result during optimization. The first is a global optimum, which results from completing continuous optimization and represents the best possible case of all the possible values of decision variables. This means that even making very small changes to the decision variables would worsen the value of the objective function. While finding this global optimum sounds ideal, it is near impossible for complex processes. It requires an immense amount of effort and time to evaluate so many minute changes to each decision variable. In addition, an actual process behaves differently than a computer model; therefore, the best case defined on paper may be different than what is best for actual operation.

Engineers want to avoid being bogged down in minute details associated with finding a global optimum. As a result, they will instead utilize discrete optimization. This means that, for any decision variable, the engineer will reanalyze the stream flowsheet and economic model for only a few specific points. The rule for selecting these points is simple: for each variable relating to equipment size, choose values that exist in the real world. While the actual optimum reactor size may be 46.857 cubic meters, it is difficult to get a reactor volume that accurate; therefore, whole number values should be tested instead. Based on the behavior of the objective function as these points change, the engineer will select the optimum. Depending on the project's time constraints, the

engineer may refine this optimum to get closer to the global optimum's value; however, that is not necessary as long as justification is given for the engineer's choice. This method ultimately makes the optimization and design processes much more creative, as there could be any number of scenarios that could be considered the best. It all depends on the engineering team's approach to the problem, because the order of the optimization steps as well as the selected process changes made can vary greatly.

There are two types of optimization that an engineer will utilize on the process design: topological and parametric. Topological deals with the type of equipment present as well as how it is arranged within the plant, and it should be considered first.

Ultimately, the engineer must keep four main considerations in mind when utilizing this type of optimization. One is to determine whether unwanted nonhazardous by-products (which cannot be sold for profit) or hazardous waste streams (which must be treated) can be eliminated. To do this, the engineer must maximize the conversion of the reactants as well as the selectivity to the desired product. In some cases, the selectivity to the desired product may decrease as the reactant conversion increases; therefore, in that case the engineer will likely prefer the high selectivity as that reduces the number of by-product streams more effectively. Another consideration is to determine if any equipment can be eliminated or rearranged. Engineers typically examine possible equipment eliminations after changing operating conditions, as this can cause some equipment from the original PFD to be redundant. Equipment rearrangements, on the other hand, are typically employed in the separation section of the process to avoid compressing gases and instead pump liquids. The third is to consider the reactor and separations sections and determine if alternative methods or configurations would work. For example, distillation is the most

common method used to separate liquids in industry because of its established technology and low energy cost compared to other separators. However, alternative methods may require implementation if the relative volatilities of the components needing to be separated are close to 1 or if the mixture requires high pressure or low temperature conditions for vapor-liquid equilibrium. The last is to consider heat integration and determine how much it can be improved. Ultimately, this potentially reduces the annual utilities cost by utilizing process streams as heating fluid.

Parametric optimization concerns operating variables, which can include temperature, pressure, and concentrations of components in streams, for a piece of equipment. The ones important to a specific system must be identified early in the optimization process in order to reduce the time and effort the problem will require. This also eliminates the possibility of investigating too many variables that will have little to no effect on the objective function. For most processes, the engineer must consider properties of the reactor, recycle, and separations sections. First, the engineer can optimize the reactor's operating conditions and single-pass conversion. The operating conditions include pressure, reactant concentrations, and temperature, which is typically constrained by the reaction's catalyst properties. Ultimately, these variable changes affect the reaction's selectivity. For the recycle streams, the engineer can optimize the recovery of unused reactants as well as the purge ratios if inert components, such as steam, are utilized as dilutants. Lastly, for the separations section, variables typically depend upon the separator type selected. In columns, the reflux ratio as well as the component recoveries in the vapor and distillate streams can vary; however, in absorbers, strippers, and extractors, the engineer can vary the amount of mass separating agent fed. Regardless

of separator type, though, the engineer should investigate changing the separator's operating pressure.

During the optimization process, engineers strategize the order in which to best complete the topological and parametric optimizations. Ultimately, this results in them either employing the top-down or bottom-up strategy. The top-down strategy consists of the engineer beginning by analyzing the big picture (thus completing topological optimization) before completing an analysis of the smaller details (thus completing parametric optimization). For example, an engineer would start the optimization process by examining the process flowsheet and asking if certain heat exchangers are actually necessary. The bottom-up strategy is the opposite; therefore, the engineer starts by investigating the smaller details of the process before looking at the process as a whole. For example, the engineer might start the optimization process by investigating the effect of changing the heating duties of the same heat exchangers. Regardless of whether the engineer employs the top-down or bottom-up strategies, he or she will reach nearly the same solution with these example starting points.

Experienced engineers, however, follow a slightly different strategy. Depending on how the optimization is progressing, he may utilize either the top-down or bottom-up strategy interchangeably. If the engineer is utilizing the bottom-up strategy and the calculations concerning specific details of the process are taking too long, he will switch back to the top-down strategy and check the broader design. Conversely, if the engineer is utilizing the top-down strategy and the analysis of the whole process gives ambiguous or indefinite results, he will switch back to the calculations for the specific process

details. Completing these switches efficiently requires the engineer to be flexible and employ engineering intuition, which is gained through experience.

III. Introduction to Process Simulation

To assist with the rigorous calculations utilized in the design and operation of a plant, a chemical engineer can utilize process simulations. These include computer programs (such as CHEMCAD, Aspen Plus, HYSYS, PRO/II, or SuperPro Designer) which can typically handle batch, semi-batch, and continuous processes with varying success. Overall, the utilization of these products by chemical engineering students is especially important in recent years. This is because companies are expecting entry-level engineers to already have knowledge of the principles common to all the simulation programs.

Ultimately, any simulation has seven input steps. The first two are preliminary steps to creating the actual process flowsheet. Therefore, the user begins the simulation by selecting the chemical components in the process from the program's component database. This is not limited only to the reactants and main products of the process; therefore, inert compounds, by-products, utilities, and waste compounds must also be included. If by chance a chemical in the process is not listed in the database, each program should include directions for the user to add them. Next, the user selects the thermodynamic model for the process. This is important for the simulator to be able to adequately predict the phase equilibria of each component in the system. Therefore, this gives the simulator access to each pure component's heat capacity, density, and critical constants. Also, in order to help the user to select the correct thermodynamic package, some simulators have "expert systems"; however, these selections are typically based on

temperatures and pressures provided by the user, so they should not be viewed as unalterable.

The next three steps involve inputting details for the process flowsheet. This begins with selecting and inputting the process topology into the simulator. This ultimately builds a virtual process flow diagram; however, it is most effective to plan the process flow diagram on paper before attempting to construct it in the simulator. Also, while most unit operations translate directly into the program, mixing points and splitting points do not. Therefore, they require “phantom” unit operations simply called “mixers” and “splitters” to represent them in a simulator. After the flowsheet is complete, the process’s feed streams must be specified. For most streams, providing temperature and pressure will be sufficient for this step. However, three feed conditions are an exception because in these cases the feed stream’s temperature and pressure are not independent. This includes saturated vapors, saturated liquids, and single component streams that have two coexisting phases. The fifth is to input the process’s equipment specifications. These allow the simulator to complete mass and energy balances on the process, and the required parameters depend upon the equipment type. For example, pumps require only one specification: either the outlet pressure or desired pressure increase. Rigorous columns, on the other hand, require multiple specifications, including one for the number of theoretical plates it contains, at least two to specify the behavior of the reboiler and the condenser, and one for the feed tray.

The last two steps finalize the flowsheet and allow it to run properly. This begins with the user deciding how the results will be displayed. Depending on what the user wants to investigate, he or she can select to display the vapor and liquid component

flowrates in each stream or any number of charts detailing equipment performance, including T-Q diagrams for heat exchangers and a composition profile for a trayed column. Finally, the last step is to select convergence criteria and run the simulation [1].

The utilization of process simulation as well as the optimization process was key to completing the following project.

Chapter 2: The Design Project

I. Base Case and Project Description

Landshark Inc. is considering implementing a styrene production process at its OM petrochemical facility. The proposed process utilizes the dehydrogenation of ethylbenzene to produce 100,000 tonnes of styrene per year with at least 99.5 weight percent purity. Landshark Inc. will sell the styrene to manufacturers interested in polymerizing it to make polystyrene packaging and foam insulation, which could potentially be profitable.

Other constraints besides the styrene product purity for the Unit 500 process were also indicated in the project description. These include component recoveries and unit temperatures and pressures. First, the toluene recovery to the overhead stream and the ethylbenzene recovery to the bottoms stream of tower T-501 must both be 99%. The styrene recovery to the bottoms stream of tower T-502 must also be 99%. In addition, the temperature in tower T-502 must be less than 125°C to avoid spontaneous polymerization of the concentrated styrene. Also, the maximum temperature in the R-501 reactor scheme is 1000 K, and the temperature drop across the reactor's length must be less than 50 K. The reactor's pressure must also be between 0.75 and 2.5 bar.

Several assumptions were also required in order to set up the Excel model of the styrene process. First, the streams behave as ideal gases and solutions; therefore, vapor-liquid equilibrium calculations in this process must utilize Raoult's Law. In addition, perfect separation between the organic liquid and aqueous phases occurs in vessel V-501, and any methane or hydrogen in the organic liquid is a dissolved gas. Finally, in the

tower section, the light key is the lightest component in the bottoms stream and the heavy key is the heaviest component in the overhead stream.

Ultimately, the base case analysis was completed and the preliminary design's economic feasibility was determined. The plant originally had a NPV of -\$320.3 M and an AE of -\$51.7 M with a MARR of 12%. This results in both a conventional and discounted payback greater than 12 years. Because of the negative NPV and a payback period longer than the project life, the project is not profitable using the preliminary design.

However, several potential changes were noted that could improve the process design. In the reactor section, the reactor type, temperatures, pressures and feed could be changed. In the separation section, the vessel pressures as well as the tower inlet temperatures and pressures could be adjusted. These all can be used as design variables. In addition, an extra tower scheme could be added to purify the benzene stream and increase the process revenue. Heat integration could also be implemented to possibly reduce the process utility costs. Improvement will be quantified based on increase in NPV, which is the objective function.

Ultimately, the changes made during the optimization process on the styrene plant are detailed in the executive summary attached in Appendix A, but the most significant changes are summarized here. First, the reactors (R-501 and R-502) were changed from isothermal to adiabatic (therefore, their names changed to R-503 and R-504). In addition, reactor R-503's volume decreased from 50 to 36 m³ and its inlet temperature was reduced from 550°C to 525°C. Also, the material of construction for the towers (T-501 and T-502) was changed from titanium to carbon steel. Lastly, tower T-503 was added to

deliver a benzene product with a higher purity. Other minor improvements were made to slightly improve the plant's NPV or to ensure the plant could operate safely. Overall, after completing the optimization process, the plant had an NPV of \$31 M and a discounted cash flow rate of return (DCFROR) of 16%. As a result, the plant was profitable and could be recommended for further development.

II. Continuing Work

All work described previously primarily pertained to the styrene process design project completed as required in the ChE 451 (the senior design course for chemical engineers) curriculum. Therefore, to fulfill the capstone requirements for the Honors College, previous work was expanded upon by investigating fluidized bed reactors as an alternative to the isothermal and adiabatic reactors investigated previously.

Chapter 3: The Fluidized Bed Reactor

I. Introduction to the Fluidized Bed Reactor

Overall, a fluidized bed reactor is one which takes advantage of fluidization theory. According to Cocco, Karri, and Knowlton of Particulate Solid Research, Inc., “particles become fluidized when an upward-flowing gas imposes a high enough drag force [due to friction imposed by the gas on the particle] to overcome the downward force of gravity”. This behavior does not occur immediately, though. Instead, this reactor begins with a packed bed. As the velocity of the gas flowing through it increases, the reactor’s pressure drop increases. However, when the drag force on the particles equals each particle’s mass, the bed fluidizes. This is referred to as the minimum fluidization velocity. Any velocity increase beyond this point can change the properties of the fluidized stream (as shown in Figure 1), but the reactor’s pressure drop will remain unchanged.

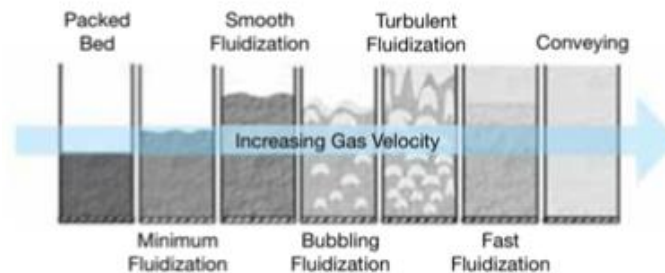


Figure 1- Stages of fluidization as gas velocity increases. Source: R. Cocco, S. B. R. Karri and T. Knowlton, "Introduction to Fluidization," *CEP Magazine*, November 2014.

However, utilization of the fluidization theory creates some unique challenges for fluidized bed reactors. First, they are much more difficult in all aspects from planning to operating; therefore, they are also difficult to scale-up. This can cause debottlenecking

issues around the reactor if higher production is necessary. In addition, because the catalyst is fluidized, some will be lost due to erosion or particle attrition. As this happens, the company must pay to replace it, and this increased cost can accumulate significantly over time.

Regardless of their challenges, though, fluidized bed reactors have several key advantages over other reactor types due to their use of fluidization. First, the heat transfer rate for a fluidized bed reactor is significantly higher than for other reactor types, like packed beds, and this can be by as much as 5 to 10 times. This also allows the fluidized bed to transfer heat produced in an exothermic reactor to a utility stream more efficiently; therefore, it can effectively maintain an isothermal profile within a 5° allowance. In addition, the fluidized catalyst allows for easy maintenance; therefore, catalyst can be added or removed from the reactor without creating any downtime [2].

II. Given Values and Assumptions for a Fluidized Bed Reactor

Ultimately, a fluidized bed reactor can be simulated as an isothermal plug flow reactor in Microsoft Excel and Pro/II software. To ensure that the reactor is actually isothermal, the reactor contains a heat exchanger to supply the heat lost in the endothermic reaction. In addition, because the catalyst bed is fluidized, a fraction of the gas fed into the reactor will not react even with an infinite-sized reactor; as a result, this fraction can be considered a bypass stream. Therefore, in all subsequent calculations, the bypass is assumed to be 10 percent of the reactor feed.

Two primary constraints were also given regarding the operation of the fluidized bed reactor. First, the fluidized bed reactor must operate within the appropriate temperature range for the catalyst being used. In this case, the catalyst was assumed to

not have changed from the one used in the preliminary styrene process design; therefore, the maximum temperature in the reactor is 1000 K. In addition, the minimum fluidization velocity must be adjusted into the superficial gas velocity for the fluidized bed reactor using a multiplier between 3 and 10.

At the beginning of the project, several values were also supplied regarding the fluidized bed configuration. This first included specifications for the catalyst. Therefore, in the following calculations and discussion, each catalyst particle is a sphere with a diameter of 300 micrometers. These particles are 100 times smaller than the catalyst particles utilized in the modelling of the isothermal and adiabatic reactors completed previously. This gives the new catalyst a smaller void fraction, which is specified as 0.45 (the isothermal and adiabatic reactor catalyst had a void fraction of 0.5). This is consistent with the fact that smaller particles can pack more efficiently, which means that there will be less empty space between particles. However, it is not likely that the difference in void fraction was the reason for using the smaller catalyst particles. Instead, it is more likely that the catalyst was selected for the fluidized bed reactor because lighter particles will fluidize easier.

In addition, specifications for the heat transfer tubes were provided. Therefore, in the following discussion, each heat transfer tube is 20 feet long with a 25 mm diameter. The overall heat transfer coefficient from the tubes to the heating medium is also defined as $200 \text{ W/m}^2\text{°C}$. In this project, the tube side stream is the utility; therefore, the length of the tubes does not also define the length of the reactor.

Lastly, specifications for the fluidized bed reactor pricing were provided. This included defining the installed cost of a fluidized bed reactor to be \$10,000 per square

meter of heat transfer surface. Based on this definition, the installed cost of the reactor is entirely dependent on the number of heat transfer tubes utilized. In addition, the bare module factor for the reactor is 2.5.

III. Algorithm for Fluidized Bed Reactor Calculations in Excel

The following discussion describes the process to replace the isothermal packed bed reactor with the fluidized bed reactor. The process was repeated to replace the adiabatic packed bed reactor with the fluidized bed reactor. For the comparison between the isothermal and fluidized bed reactors, the feed stream (which in Appendix B1 and B5 is shown as stream 9) has the same flowrate and composition as well as the same inlet temperature and pressure of 550°C and 190 kPa, respectively. The actual comparison between the reactor types will be focused on annual operating cost as well as outlet stream composition and pressure drop. This section will only focus on the latter two.

As stated previously, it was assumed that 10 percent of the feed bypasses the fluidized bed reactor; therefore, the first step of the calculations was to separate the 10 percent of bypass from the 90 percent of reactor feed. At this point, it was assumed that the stream splits perfectly to keep the concentrations of all components (including water, ethylbenzene, styrene, benzene, and toluene) the same in both the bypass and the feed stream.

Next, it was assumed that the process would contain 1 large reactor with a volume of 250 cubic meters (equal to the entire catalyst volume). This was an arbitrary decision that could easily be changed to multiple reactors in parallel with smaller, equal volumes. Because the composition of the reacting stream changes as it progresses through the reactor, calculations were done for 10 reactor intervals of 25 cubic meters each. Also,

because this was simulated in Excel, complicated and more realistic thermodynamic packages were not able to be utilized; therefore, it was assumed that the ideal gas law applied to all streams in the process.

To continue the calculations investigating the outlet stream composition and the pressure drop, the change in the number of moles of each component per hour was first able to be tabulated using the 4 reaction rate laws given previously in the project assignment (shown in Appendix D1). Because the steam present in the reactor was a diluent, the number of moles of water in the reactor was constant. This determined the pressure increase for each reactor interval due to an increase in the number of moles in the reactor. However, this pressure increase was ultimately countered and overcome by a larger pressure drop calculated using the Ergun equation.

The Ergun equation requires the length of each reactor interval. However, the actual dimensions of the reactor were originally unknown and needed to be calculated. In order to achieve this, the calculations described next were completed with the assumption that, for each of the reactor intervals, the inlet stream defined properties such as the density of each component as well as the minimum fluidization velocity of the reacting stream. Based on these assumptions, the length and cross-sectional area of the reactor varied with each interval.

The calculations to determine reactor length can be split into two smaller subsections with distinct goals. Ultimately, the first goal was to determine the superficial gas velocity in the reactor. This first required determination of the minimum fluidization velocity in the reactor, which could be simply calculated using the Archimedes and Reynolds numbers (shown in Equations 1 and 2).

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

$$Re = \frac{u_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408Ar]^{0.5} - 33.7$$

Equation 1 and 2- Equations for the Archimedes number and Reynolds number. In this case, Ar is the Archimedes number, Re is the Reynolds number, d_p is the particle diameter, ρ_s is the catalyst density, ρ_g is the gas density, μ_g is the gas viscosity, and g is the acceleration due to gravity.

Upon closer investigation, it was clear that only one variable required for these equations was absent from the project description: the density of the reacting gas. To find this, the ideal gas law was first required to determine the density in each interval of each component in the reacting stream. Then, the overall gas density in the reactor interval was calculated using a weighted average. Once the minimum fluidization velocity in each interval was determined, it required adjustment using a multiplier to determine the superficial velocity of the gas. As stated previously, this multiplier must be between 3 and 10; therefore, for these calculations, the value of 6.5 was arbitrarily selected as it is exactly in the middle of the available range.

The second goal was to determine the reactor's cross-sectional area and length. This was done using the volumetric flowrate, which was calculated using the ideal gas law for each interval. Then, knowing the superficial gas velocities calculated previously, the cross-sectional area for each interval was calculated. This was then used to find the length based on a reactor volume of 250 cubic meters.

Ultimately, these calculations resulted in 11 different possibilities for the reactor's length and cross-sectional area due to the 11 different superficial velocities calculated.

However, the length, cross-sectional area, and superficial velocity calculated for the final interval (right before the stream exits the reactor) was selected for the entire reactor because it allows the accommodation of the largest volumetric flowrate of reacting gas. These values satisfy the variables of the Ergun equation which had not been supplied in the project description.

IV. The Selection of the Fluidized Bed Reactor Configuration

Completing the calculations discussed in the previous section ultimately resulted in a fluidized bed reactor with a cross-sectional area of 198 m^2 and a length of 1.3 meters. The stream passing through this reactor also experienced a pressure drop of 56.5 kPa (from 190 to 133.5 kPa). Overall, this pressure drop was not unreasonable. This was because, in previous calculations completed during the styrene optimization project, the pressure of the stream leaving the reactor section could be as low as approximately 110 kPa without negatively impacting the process's performance. This can be seen in stream 12 (shown in Appendix B5) in the optimized styrene process with the adiabatic reactors.

However, the large cross-sectional area of 198 m^2 (and therefore a diameter of nearly 16 meters) was cause for alarm in this case. This diameter is approximately twice as large as the diameter of each individual large tower in the T-502 scheme. In the base case (with isothermal reactors), each tower with T-502 specifications had a diameter of 7.1 m. Likewise, Appendix B8 showed that in the optimized case (with adiabatic reactors), each T-502 tower had a diameter of 9.0 m. As a result, the reactor's large diameter seemed unreasonable in comparison.

The only reasonable remedy to the issue with the large reactor diameter was to split it into multiple reactors with smaller, equal volumes (which sum to the 250 m^3

required) in parallel. If there were 2 reactors in the scheme, each would have a volume of 125 m^3 and handle 45% of the stream 9 flowrate. Completing the previously discussed calculations with these values gave each reactor a cross-sectional area of 99.2 m^2 , which means that the diameter of each was 11.2 m. This is still larger than the diameters in the T-502 scheme.

Therefore, a scheme with 3 reactors needed to be investigated. If there were 3 reactors, each would have a volume of 83.3 m^3 and handle 30% of the stream 9 flowrate. These values resulted in each reactor having a cross-sectional area of 66.1 m^2 . This means that the diameter for each reactor was 9.2 m, which is very close to the diameter of the towers in the T-502 scheme. Therefore, the configuration with 3 fluidized bed reactors in parallel was selected, and it maintained the same length and pressure drop as the one large fluidized bed reactor. In addition, it was assumed that the fluidized bed reactors used nC36 as a utility to maintain an isothermal profile. This allowed the number of tubes required in each reactor to be calculated.

Chapter 4: Comparing Reactor Types Based on EAOs

Overall, in order to determine which reactor (isothermal, adiabatic, or fluidized bed) was best for the styrene production process, it was necessary to define the quantitative metric by which the 3 would be compared. In this project, it was possible that net present value (NPV) could have been chosen, as this was the metric previously utilized during process optimization. However, a simpler metric to use was the equivalent annual operating cost, or EAO, which takes into account only the reactor and its associated utility streams.

In order to calculate the EAO of each reactor, it was first necessary to calculate the capital investment associated with each reactor scheme. In the case of the isothermal and adiabatic reactors, there were 2 schemes with 5 reactors each. This is shown as R-501a-e and R-502a-e for isothermal reactors in Appendix B1 and R-503a-e and R-504a-e for adiabatic reactors in Appendix B5. This was then plugged into the capital recovery equation shown below (the capital investment is the present value, or P variable) to find the annual equivalent of the capital investment. This assumed that the capital investment could be modelled as an equal payment series. For the styrene production process, the plant life (N) is 12 years and the interest rate (i) is 12 percent.

$$A = P \left[\frac{i(1+i)^N}{(1+i)^N - 1} \right]$$

Equation 3- The capital recovery equation where the capital investment is the present value (P). In this case, i is the interest rate and N is the plant life.

Then, the yearly operating cost for each reactor was determined. In this case, it was assumed that there was no annual cost for the refrigerant nC36 used by the

isothermal and fluidized bed reactors. Therefore, only the utility which provided the energy for the reactor- in this case, the natural gas used in the fired heater- needed to be taken into account. Because this was already on a yearly basis, no adjustment needed to be made to it.

Ultimately, in order to enable ease of calculation, the fluidized bed reactor must be compared to the isothermal reactor from the base case styrene production process and the adiabatic reactor from the optimized production process. This is due to the fact that the first optimization step completed on the styrene process was to choose between the isothermal and adiabatic reactor types. Because the adiabatic reactor was deemed better, it was present in all the subsequent optimization steps. The results are shown in Tables 1 and 2 below.

Table 1- EAOCs calculated for the isothermal and fluidized bed reactors the base case styrene process

EAOE of Reactor in the Base Case Styrene Process	
Isothermal	\$9,736,000
Fluidized Bed (each with 159 tubes)	\$4,525,000

Table 2- EAOEs calculated for the adiabatic and fluidized bed reactors in the optimized styrene process

EAOE of Reactor in the Optimized Styrene Process	
Adiabatic	\$18,466,000
Fluidized Bed (each with 165 tubes)	\$8,672,000

Ultimately, no further optimization was able to be completed on the fluidized bed reactors because the only variable affecting the calculated EAOE was the number of heat transfer tubes, which changed the heat transfer area. This, however, was set by the reaction as well as the selected reactor utility. Ideally, though, more detailed calculations

for the EAOB would allow the velocity multiplier, the reactor utility, and the reactor inlet temperature and pressure to be optimized.

It was very clear based on the simplified calculations that the fluidized bed reactors were the best option to minimize the reactor cost in the styrene production process. This was most likely due to the fact that the 3 fluidized bed reactors could take the place of 10 isothermal or adiabatic reactors; therefore, they greatly reduced the capital investment for the reactors. Ultimately, the requirement of fewer actual reactors in the process was due to the fact that, by virtue of the fluidized process stream, the fluidized bed reactors have more efficient heat transfer.

However, it must be noted that, while the EAOB of the adiabatic reactors is larger than that of the isothermal reactors, isothermal reactors are not necessarily better. This is due to the fact that adiabatic reactors actually have a higher yield of styrene from ethylbenzene (58 percent for adiabatic reactors versus 50 percent for isothermal). This resulted in a decrease in the cost of raw materials which counteracted and overcame the increased reactor cost. Ultimately, this shows that, in order to be more definitive about which reactor was superior, it would be better to create a clearer comparison between the three. This could be done by setting the conversion or selectivity within the reactors constant and solving for the equivalent annual operating cost again. In addition, it would likely be better to compare the net present value of the optimized styrene process with the different reactor types implemented. Without time constraints, these would be the next steps to continue the project.

Chapter 5: Conclusion

Ultimately, this thesis began with a discussion about chemical engineering design, process optimization, and simulation. These were necessary to complete the ChE 451 design project, which was to create an optimized styrene process given a base case. During the design project, isothermal and adiabatic reactors were investigated. However, this work was expanded upon by investigating fluidized bed reactors as an alternative.

The theory behind fluidized bed reactors was discussed before the fluidized bed reactor calculations were detailed. Overall, the fluidized reactor was simulated in Microsoft Excel. The calculation algorithm can be summarized with three main equations: the Archimedes and Reynolds number equations (which helped to calculate the minimum fluidization velocity in the reactor) and the Ergun equation (which determined the reactor's pressure drop along its length). In the end, these calculations resulted in a scheme of 3 fluidized bed reactors with volumes of 83.3 m³ in parallel.

Lastly, the equivalent annual operating costs (EAOCs) of the isothermal, adiabatic, and packed bed reactors were calculated. When compared to the isothermal and adiabatic reactors, the fluidized bed reactors were found to have approximately half the associated costs. This was likely because the fluidized bed reactor scheme only contained three reactors while the isothermal and adiabatic schemes each contained ten; therefore, the capital investment required for the fluidized bed reactors is much smaller. However, these calculations were greatly simplified. As a result, to get a more accurate picture of the reactor comparison, the conversion or selectivity in all the reactors should be set constant and the EAOCs should be calculated again. The net present value of the styrene process with the different reactor types could also be compared.

Appendices

Appendix A – Styrene Process Optimization Design Report (written with Seth Gray and Mitch Sypniewski in ChE 451, Fall 2018)

I. Introduction

Landshark Inc. is considering implementing a styrene production process at its OM petrochemical facility. The proposed process utilizes the dehydrogenation of ethylbenzene to produce 100,000 tonnes of styrene per year with at least 99.5 weight percent purity. Landshark Inc. will sell the styrene to manufacturers interested in polymerizing it to make polystyrene packaging and foam insulation, which could potentially be profitable.

Our engineering team received a preliminary design and was instructed to first complete a base case analysis and determine economic feasibility. We found that the plant had a net present value (NPV) of -\$320.3 M. Because this NPV is negative, our team will require information about the other sections of the plant (such as a styrene polymerization section, if it exists) to make an accurate recommendation regarding the project. Assuming a later section of the OM facility does polymerize 100,000 tonnes of styrene per year, the NPV based on buying the styrene at market value is -\$1.4 B; therefore, under these conditions, Landshark Inc. should pursue the project further even in its current form. If Landshark Inc. does not polymerize styrene, though, they should not pursue the project further with the current design as it would only increase company debt.

After completing base case analysis, we then investigated changes proposed by management as well as other optimizations as we saw fit. These changes gave the plant an NPV of \$31 M, which indicates that the updated design can turn a profit and the

project should undergo further consideration regardless of whether or not the OM facility polymerizes styrene.

II. Base Case

Our engineering team modeled the base case of Landshark, Inc.'s preliminary design in Microsoft Excel. We simulated the same design in Pro/II to utilize more complicated and realistic thermodynamic relationships in our calculations. We then compared those results to the Excel simulation, which assumed that the streams behave as ideal gases and solutions. In Pro/II, we used the SRK-SimSci thermodynamic model based on the path our system follows in the thermodynamic flowsheet (see Appendix C11). The tower T-502 scheme, however, was simulated using the ideal thermodynamic method.

Our team found that the preliminary design as given to us by management had a NPV of -\$320.3 M and an annual equivalent (AE) of -\$51.7 M with a 12% minimum acceptable rate of return (MARR). This results in both a conventional and a discounted payback period greater than 12 years. Because the project had a negative NPV and a payback period longer than the project life, the project is not profitable with the preliminary design. However, with changes it could become more lucrative.

After inspection, several process parameters fell outside of normal operating conditions defined in *Analysis, Synthesis, and Design of Chemical Processes* by Turton et al. We then analyzed whether each of these conditions was justified. First, moving sequentially through the plant, reactors R-501 and R-502 had both high temperature and non-stoichiometric feed. These are justified because the steam present in the feed improves reactor conversion and provides heat to both fuel the reaction and keep all

components in the gas phase. The low pressure of the towers T-501 and T-502 and the vessels V-502 and V-503 are justified by the need of a gas phase for vapor-liquid equilibrium and the lack of pumps or valves between the towers and vessels. The large log mean temperature differences of heat exchangers E-501, E-502, E-503, and E-505 are justified because the utilities defined in the base case (either high pressure steam or cooling water) are required to vaporize or cool each exchanger's respective stream. Compressor C-501 also has a pressure ratio of 6; however, unlike the previous parameters, this is not justified and must be changed for the optimized case.

Finally, we utilized sensitivity analysis (shown in Appendix C1) to determine which parameters had the greatest effect on NPV. As can be seen in the figure, the styrene price and the raw materials cost varied the most. Due to this observation, we decided to focus on reducing the raw materials cost.

III. Notes about Sign Conventions for Optimization

The engineering team used discrete optimization when trying to make improvements to the styrene production process. When referring to an increased cost, the NPV contribution is becoming more negative.

IV. First Change: Reactor Type

The first change we investigated was replacing the original isothermal reactors with adiabatic reactors. We treated isothermal reactors as heat exchangers, since the reacting stream will only undergo a pressure drop within the reactor. We also treated adiabatic reactors as vessels, since the reacting stream will undergo both a temperature and a pressure drop within the reactor. Ultimately, the objective in doing this was to decrease the raw materials cost by increasing the overall yield of styrene.

Appendix C2 shows an economic comparison of the process after implementing each type of reactor. Notice that the inlet temperature of the adiabatic reactor R-503 is 25°C lower in comparison to the original isothermal reactor. This adjustment was made because preliminary design conditions stipulated that the temperature drop in each reactor must be less than 50°. The choice of 525°C resulted in a temperature drop of 49.86°. Lowering the temperature further would result in a lower NPV because it increases the fixed capital investment as well as the annual cost of raw materials and utilities. Overall, these changes improved the NPV by approximately \$56 M. Appendix C2 shows the breakdown of the most notable cost contributions (raw materials, utilities, and fixed capital investment).

The largest contribution to the improved NPV was the decrease in the cost of raw materials. This was due to a lower single pass conversion of ethylbenzene in the reactor section (57% to 42%), which ultimately resulted in a larger ethylbenzene recycle stream and a higher overall yield of styrene (50% to 58%). The elimination of the original isothermal reactor also increased NPV by saving approximately \$2 M in heating utility costs. The almost 4,800 kmol/hr increase in the steam utility required to heat the reactor R-503 effluent (stream 12) to the inlet temperature of R-504 counteracted but did not overcome the cost savings.

The contribution of the FCI to the project's NPV is primarily attributed to three different points in the process. Firstly, the adiabatic reactors R-503 and R-504 have larger equipment equipment cost attributes, which are related to capacity and are reported in square meters for heat exchangers and cubic meters for vessels. In this process, the vessel volume is the same as the catalyst volume- 50 m³ - while the heat exchanger area required

is smaller (and it stores the required volume of catalyst in its shell.) Therefore, the equipment with the larger equipment cost attributes (in this case, the vessels) is more expensive. Second, the duty (and therefore the size) of the fired heater increases when the process implements an adiabatic reactor. This is due to the increased steam utility in heat exchanger E-503. Lastly, the cost of the tower T-502 scheme increases because the number of towers required increases from 4 to 5. This is due to the lower single pass conversion of ethylbenzene in the reactor sections; therefore, this leaves a larger amount of ethylbenzene present in T-502, and the higher flowrate requires a larger tower volume.

Overall, this decision is based on a comparison between the preliminary isothermal reactor and the optimized adiabatic reactor. If given more time, the engineering team would pursue optimization of the isothermal reactor for a more thorough decision concerning which reactor type is preferable.

V. Second Change: Reactor Conditions

The second change we investigated was changing the volume and pressure of reactor R-503 and the volume of R-504. Similarly to the change from isothermal to adiabatic reactors, the objective in doing this was to decrease the raw materials cost (by increasing the overall yield of styrene). Overall, these changes improved the NPV by approximately \$60 M. A breakdown of the most notable cost contributions (raw materials, catalyst, utilities, and fixed capital investment) is shown in Appendix C3.

The most significant change in the reactor scheme was adjusting the volumes of R-503 and R-504 from 50 to approximately 36 m³. In both reactors this resulted in a slight decrease in single-pass conversion and an increase in the selectivity of ethylbenzene, as seen in Appendices B4-B7. The changes in conversion and selectivity

ended up increasing the yield of styrene from the reactors (from 58% to 68%). This in turn decreased the required feed of ethylbenzene by 28.4 kmol/hr, which ultimately decreased the raw materials cost by \$22 M per year. Since the catalyst volume is proportional to the reactor volume, this change accompanied a decrease in the catalyst cost of \$2.5 M per year.

An insignificant change made to the reactor scheme was changing the inlet pressure to R-503 from 190 to 187.5 kPa. This only increased the NPV by approximately \$1 M due to the given rate law equations, which are in terms of partial pressures.

VI. Third Change: Materials of Construction

The third investigation was on the materials of construction of the towers and reactors. The preliminary tower design specified using titanium, which is very expensive. Carbon steel is usable at the towers' operating conditions (vacuum pressures and $T < 125^{\circ}\text{C}$) and is about 11% the cost of titanium. The outsides of the towers will need to be epoxied or painted to prevent atmospheric corrosion.

The base case reactors were made of 316 stainless steel which is susceptible to hydrogen embrittlement and hydrogen blistering. This is where atomic hydrogen diffuses into a dislocation in a metal and bonds with another atomic hydrogen to form a gas. The gas expands and damages equipment, causing it to need to be replaced more frequently [3]. Due to the mechanism of ethylbenzene dehydrogenation, atomic hydrogen will be present in the reactors. We changed the material of construction to nickel alloy clad, which is less susceptible to hydrogen embrittlement and hydrogen blistering, since it is also operable under the reactors' conditions ($T < 600^{\circ}\text{C}$ and $P < 200$ kPa). This change

slightly decreased the NPV by increasing the FCI. This occurred because nickel alloy clad is more expensive than stainless steel.

Ultimately, changing the material of construction of the towers and reactors increased our NPV by \$165 M. The main contribution to this was a decrease in the FCI because the decreased tower cost greatly outweighed the increased reactor cost, as shown in Appendix C8.

VII. Fourth Change: Extra Tower to Purify Benzene Stream

The fourth change that was analyzed was the addition of a benzene/toluene distillation tower (T-503). The benzene and toluene byproduct stream entered T-503 at 50°C and 200 kPa. Tower T-503 separated the benzene and toluene to deliver benzene with 99.5 mole percent purity to the bottoms. With this high purity, Landshark Inc. could sell the benzene at full price, therefore increasing the revenue of the plant from \$239 M to \$253 M. This outweighs the \$0.5 M decrease in FCI. This ultimately increased NPV by \$56 M.

VIII. Fifth Change: Heat Integration

Due to the recent decrease in the market value of utilities, the engineering team only focused on implementing heat integration in one section of the process. In the preliminary design, high pressure steam (HPS) heated and vaporized stream 2 in heat exchanger E-501. The effluent from reactor R-502, or stream 12, flowed directly into heat exchanger E-503 where it cooled through interaction with cooling water (CW) and exited as stream 13. The preliminary design PFD (Appendix B1) shows this setup.

The proposed changes shown in the optimized design PFD (Appendix B5) resulted in an elimination of the HPS utility in E-501 and a reduction in the CW required in E-503. In the new design, the effluent stream 12 from reactor R-504 (previously called R-502 in the base case) redirects to the utility side of E-513 (previously E-501). Since it now serves as the heating fluid, its temperature decreases in the heat exchanger and exits as stream 36. This flows into E-503 where it cools further to become stream 13. Overall, this improved the NPV by approximately \$4 M. Appendix C9 shows the breakdown of the most notable cost contributions (raw materials, utilities, and fixed capital investment).

IX. Sixth Change: Compressor Adjustments

In the base case, the pressure ratio across compressor C-501 was 6. For safe operating conditions the pressure ratio needed to be decreased to below 3. To achieve this, the engineering team looked into using multi-stage compression. When adding a second compressor (C-502) with an interstage cooler, the pressure ratio decreased to approximately 2.45 across both C-501 and C-502. We accepted this change because it is under the threshold for safe operation. With the addition of a second compressor (C-502) and a heat exchanger (E-512), the utilities and FCI decreased compared to the base case. This increased the NPV by \$11 M.

X. Summary

The economic data for the optimized case results in an NPV of \$31 M, a discounted cash flow rate of return (DCFROR) of 16%, and an annual equivalent (AE) of \$4.93 M. Provided below in Appendix C10 is a comparison of the optimized case and the base case. The DCFROR for the base case has been marked as N/A since it could not be calculated.

XI. Process Safety Considerations

Overall, one of the main concerns for process safety will be keeping high temperature vapors and steam away from employees. If exposure to high temperature lines is likely, maintenance staff and operators should wear proper PPE. Otherwise, during the design process, engineers can protect employees by consciously attempting to put high temperature process and steam lines away from expected high traffic areas. In addition, the temperatures throughout the process are higher than the flash points of each component. Therefore, there will need to be measures put into place to avoid ignition sources. Also, since the reaction is endothermic, runaway reactions will not be a concern. However, isolating the reactors, where temperatures of the streams are extremely high, would also be advisable. This alleviates the danger of burns if there is a rupture in piping or equipment.

The other main process safety concern noted was limiting exposure to the chemicals in the process. In the case of a spill, people exposed to high concentrations of chemical vapor must use self-contained respiratory devices because components in the process can act as lung irritants and asphyxiants. Also, proper ventilation should be in place in all areas where spills are likely to occur.

XII. Sensitivity Scenarios

The three parts of this process that were most susceptible to change were the prices of ethylbenzene, styrene, and utilities; therefore, the team focused on formulating scenarios for changes in these variables. The following changes would affect the optimized case defined above.

First, the team investigated ethylbenzene and styrene scenarios. If the price of ethylbenzene decreases, then the team would not have to focus so much on maximizing the overall yield of styrene. Also, if the price of ethylbenzene increases or the price of styrene decreases, it might not be profitable to produce the styrene. It may be better to simply purchase the styrene. Lastly, if the price of styrene increases, the profitability of producing the styrene on-site would increase.

In addition, utility costs are susceptible to change. If the cost of utilities were to increase, heat integration would need further investigation and implementation. This would allow the plant to minimize necessary utilities. If the cost of utilities were to go down, little would change in the optimized design process.

XIII. Conclusions

Given specifications of 100,000 tonnes of styrene produced per year with a purity of at least 99.5 wt%, the engineering team determined the economic viability of producing styrene from the dehydrogenation of ethylbenzene. The NPV of the base case was -\$320.2 M.

However, after the proposed changes, the NPV of the optimized case was \$31 M. Therefore, we recommend the optimized case undergo further investigation and optimization. Our recommendations include investigating different inlet temperatures and pressures in tower T-503, adding more heat integration, and improving vessel V-501. After finishing optimization, Landshark Inc. could begin to discuss options for buying the process equipment from contractors, thus reducing the design inaccuracy due to the pricing calculations.

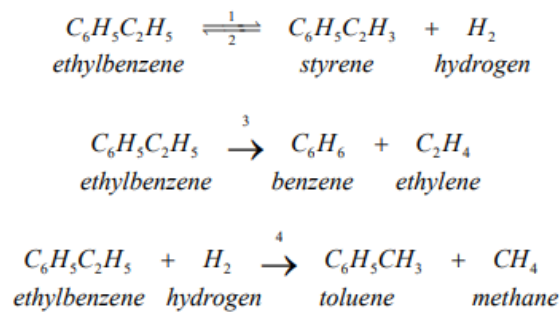
2. Base Case Stream Table

Stream No.	1	2	3	4	5	6	7	8	9
Temperature (°C)	136	117	225	159	800	800	800	800	550
Pressure (kPa)	205	205	190	600	565	565	565	190	190
Vapor Mole Fraction	0	0	1	1	1	1	1	1	1
Total Flow (kg/h)	26430	45962	45962	90742	90742	28288	62454	62454	108416
Total Flow (kmol/h)	250	434	434	5037	5037	1570	3467	3467	3901
Comp. Flow (kmol/h)									
Water	0	0	0	5037	5037	1570	3467	3467	3467
Ethylbenzene	245	427	427	0	0	0	0	0	427
Styrene	0	1.2	1.2	0	0	0	0	0	1.2
Hydrogen	0	0	0	0	0	0	0	0	0
Benzene	2.5	2.5	2.5	0	0	0	0	0	2.5
Toluene	2.5	3.1	3.1	0	0	0	0	0	3.1
Ethylene	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0
Stream No.	10	11	12	13	14	15	16	17	18
Temperature (°C)	550	575	575	270	180	65	65	65	65
Pressure (kPa)	180	165	147	132	117	102	102	102	102
Vapor Mole Fraction	1	1	1	1	1	0	1	0	0
Total Flow (kg/h)	108416	108416	108416	108416	108416	108416	3738	43077	61600
Total Flow (kmol/h)	4023	4023	4080	4080	4080	4080	219	442	3419
Water	3467	3467	3467	3467	3467	3467	47	0	3419
Ethylbenzene	273	273	186	186	186	186	0.9	185	0
Styrene	98	98	121	121	121	121	0	121	0
Hydrogen	64	64	58	58	58	58	56	1.5	0
Benzene	28	28	62	62	62	62	2.1	60	0
Toluene	35	35	65	65	65	65	0.8	64	0
Ethylene	25	25	60	60	60	60	51	8.4	0
Methane	32	32	62	62	62	62	59	2.7	0
Stream No.	19	20	21	22	23	24	25	26	27
Temperature (°C)	227	65	50	121	91	123	700	50	123
Pressure (kPa)	240	60	40	60	25	55	555	200	200
Vapor Mole Fraction	1	0	0	0	0	0	1	0	0
Total Flow (kg/h)	5354	43077	9430	32032	19532	12500	28288	9430	12500
Total Flow (kmol/h)	247	442	110	304	184	120	1570	110	120
Water	47	0	0	0	0	0	1570	0	0
Ethylbenzene	1.0	185	1.8	183	182	0.6	0	1.8	0.6
Styrene	0	121	0	121	1.2	119	0	0	119
Hydrogen	58	1.5	0	0	0	0	0	0	0
Benzene	14	60	49	0	0	0	0	49	0
Toluene	5.5	64	59	0.6	0.6	0	0	59	0
Ethylene	59	8.4	0	0	0	0	0	0	0
Methane	62	2.7	0	0	0	0	0	0	0
Stream No.	28	29	30	31					
Temperature (°C)	65	91	50	63					
Pressure (kPa)	200	205	40	40					
Vapor Mole Fraction	0	0	1	1					
Total Flow (kg/h)	61600	19532	1615	5354					
Total Flow (kmol/h)	3419	184	29	247					
Water	3419	0	0	47					
Ethylbenzene	0	182	0	1.0					
Styrene	0	1.2	0	0					
Hydrogen	0	0	1.5	58					
Benzene	0	0	11	14					
Toluene	0	0.6	4.7	5.5					
Ethylene	0	0	8.2	59					
Methane	0	0	2.7	62					

Table 1: Base case stream table as calculated for ChE 451 (all flowrates are in kmol/h)

3. Base Case Process Description

Fresh liquid ethylbenzene at 136°C and 205 kPa (stream 1) is combined with a recycle of liquid ethylbenzene (stream 29) to form a feed mixture (stream 2). This then enters heat exchanger E-501 which utilizes high pressure steam to vaporize the stream and increase its temperature to 225°C (stream 3). The stream experiences a pressure drop of 15 kPa through the heat exchanger, which is typical of all of the heat exchangers in the process. The vaporized stream 3 is mixed with an adequate amount of high-pressure steam (stream 8) to form stream 9. This stream is then fed to reactor R-501a-e at a temperature of 550°C and a pressure of 190 kPa. The reactor consists of a catalytic bed and has 4 reactions that occur:



For the equations above, p_i is the partial pressure of component I in Pa, T is the temperature in K, the activation energy is in J/mol, and the rate is in mole/(m³ catalyst * second).

The effluent (containing ethylbenzene, styrene, hydrogen, benzene, ethylene, toluene and methane) coming from the reactor at 550°C and 179.9 kPa (stream 10) is then sent to a heat exchanger E-502 that increases the temperature to 575°C. Stream 11 coming from E-502 enters the second reactor R-502a-e and undergoes the same reactions shown previously. The 8-component vapor stream exiting the reactor (stream 12) is fed to

a series of three heat exchangers (E-503, E-504, and E-505, which use high pressure steam, low pressure steam, and cooling water utilities respectively). Here the vapor is cooled and partially condensed into a liquid/vapor mixture at 65°C and 102.2 kPa (stream 15). This mixture is then fed to a 3-phase separator, V-501, where it separated into three streams: the vapor stream (stream 16), containing all the aqueous and organic components in the inlet stream, the organic liquid stream (stream 17), and a water stream (stream 18). The vapor stream is mixed with the fuel gas coming out of reflux drum V-502 (stream 30) to form stream 31. Stream 31 is then fed to compressor C-501 which increases the temperature and pressure to 227°C and 240 kPa (stream 19). These are the conditions at which the stream is sold as fuel gas. The water stream is fed to pump P-501A/B where the pressure is increased to 200 kPa and treated as wastewater. The organic liquid stream goes through a valve and comes out at 60 kPa (stream 20). Stream 20 is then fed onto tray 4 of the first tower T-501, which has 18 stages and operates at 65°C and between 40 and 60 kPa. This tower has a reboiler, E-506, which uses a low-pressure steam utility. The column produces a bottoms stream (stream 22) which recovers 1% of the toluene and 99% of ethylbenzene in stream 20.

The vapor stream from the top of T-501 is condensed in heat exchanger E-507 using cooling water and sent to Reflux Drum V-502. Here the vapor and liquid phases are separated into streams 30 and 21 respectively. The vapor stream 30 is combined with the fuel gas. The liquid benzene/toluene byproduct (stream 21) is sent to pump P-504A/B where the pressure is increased to 200 kPa. Stream 22 (bottoms product from T-501) is fed to tray 28 of T-502 where further separation is accomplished. T-502 contains 68 total stages, and it operates between 25 and 55 kPa. It also has a reboiler (E-508), which uses

low pressure steam. The vapor product from the top of the T-502 condenses in heat exchanger E-509, using cooling water, before it goes through reflux drum V-503. The liquid stream then goes through pump P-503A/B where its pressure decreases to 25 kPa (stream 23). Stream 23 is then sent through P-506A/B where the pressure is increased to 205 kPa before it is recycled and combined with stream 1. The bottoms of T-502 in stream 24 are sent to P-505A/B where it undergoes a pressure increase to 200 kPa to become stream 27. This is the final pure styrene product (with a 99.5 mass percent purity) flowing at a rate of 100,000 tonnes per year.

The only other inlet stream is low pressure steam fed to the fired heater H-501 at 159°C and 600 kPa (stream 4). It is heated in H-501 to 800°C in stream 5 where it is then split into streams 6 and 7. Stream 7 goes through a valve where there is a 375 kPa pressure drop before going into stream 8 which combines with stream 3. Stream 6 is fed to heat exchanger E-502 and is used to heat the first reactor effluent (stream 10) to 575°C.

4. Optimized Case Process Description

Fresh liquid ethylbenzene at 136°C and 205 kPa (stream 1) is combined with a recycle of liquid ethylbenzene (stream 29) to form a feed mixture (stream 2). This then enters heat exchanger E-513 which utilizes stream 12 from reactor to vaporize the stream and increase its temperature to 225°C (stream 3). The stream experiences a pressure drop of 15 kPa through the heat exchanger, which is typical of all of the heat exchangers in the process. The vaporized stream 3 is mixed with an adequate amount of high-pressure steam (stream 8) to form stream 9. This stream is then fed to reactor R-503a-e at a temperature of 525°C and a pressure of 187.5 kPa. The reactor consists of a catalytic bed and has 4 reactions that occur:

The effluent (containing ethylbenzene, styrene, hydrogen, benzene, ethylene, toluene and methane) leaves the reactor at 483°C and 164 kPa (stream 10). It is then sent to heat exchanger E-502 where the temperature increases to 575°C. Stream 11 coming from E-502 enters the second reactor, R-504a-e, and undergoes the same reactions shown previously. An 8-component vapor stream exits the reactor (stream 12) and is then used as the utility in E-513. Stream 12 goes through E-513 and become stream 36 which is fed to a series of three heat exchangers (E-503, E-504, and E-505, which use high pressure steam, low pressure steam, and cooling water utilities respectively). Here the vapor is cooled and partially condensed into a liquid/vapor mixture at 65°C and 68 kPa (stream 15). This mixture is then fed to a 3-phase separator, V-501, where it separated into three streams: the vapor stream (stream 16), containing all the aqueous and organic components in the inlet stream, the organic liquid stream (stream 17), and a water stream (stream 18). The vapor stream is mixed with the fuel gas coming out of reflux drum V-

502 (stream 30) to form stream 31. Stream 31 is then fed to compressor C-501 which increases the temperature and pressure to 157°C and 98 kPa (stream 34). Stream 34 is sent to an interstage cooler E-512 where it cools the stream to 63°C (stream 35). Stream 35 is then fed to compressor C-502 where its temperature and pressure are increased to 157°C and 240 kPa (stream 19). These are the conditions at which the stream is sold as fuel gas in stream 19. The water stream (stream 18) is fed to pump P-501A/B where the pressure is increased to 200 kPa and treated as wastewater. The organic liquid stream goes through a valve and comes out at 60 kPa (stream 20). Stream 20 is then fed to tower T-501 which has 32 stages and operates at 65°C and between 40 and 60 kPa. This tower has a reboiler, E-506, which uses a low-pressure steam utility. The column produces a bottoms stream (stream 22) which recovers 1% of the toluene and 99% of ethylbenzene in stream 20.

The vapor stream from the top of T-501 is condensed in heat exchanger E-507 using cooling water and sent to Reflux Drum V-502. Here the vapor and liquid phases are separated into streams 30 and 21 respectively. The vapor stream 30 is combined with the fuel gas. The liquid benzene/toluene byproduct (stream 21) is sent to pump P-504A/B where the pressure is increased to 200 kPa (stream 26). Stream 26 is then fed to tower T-503 where the overhead product (Stream 32) is 99.5 mole % benzene. The overhead is condensed in exchanger E-511 and sent to Reflux Drum V-504. After V-504 the stream is sent through pump P-507A/B where stream 32 is sold as benzene. The bottoms for T-503 is the Toluene stream in stream 33 that is sold. The reboiler for tower T-503 is E-510. Stream 22 (bottoms product from T-501) is fed to tray 28 of T-502 where further separation is accomplished. T-502 contains 68 total stages, and it operates between 25

and 55 kPa. It also has a reboiler (E-508), which uses low-pressure steam. The vapor product from the top of T-502 condenses in heat exchanger E-509, using cooling water, before it goes through reflux drum V-503. The liquid stream then goes through pump P-503A/B where its pressure decreases to 25 kPa (stream 23). Stream 23 is then sent through P-506A/B where the pressure is increased to 205 kPa before it is recycled and combined with stream 1. The bottoms of T-502 in stream 24 are sent to P-505A/B where it undergoes a pressure increase to 200 kPa to become stream 27. This is the final pure styrene product (with a 99.5 mass percent purity) flowing at a rate of 100,000 tonnes per year.

The only other inlet stream is low pressure steam fed to the fired heater H-501 at 159 °C and 600 kPa (stream 4). It is heated in H-501 to 800 °C in stream 5 where it is then split into streams 6 and 7. Stream 7 goes through a valve where there is a 375 kPa pressure drop before going into stream 8 which combines with stream 3. Stream 6 is fed to heat exchanger E-502 and is used to heat the first reactor effluent (stream 10) to 575 °C.

5. Optimized Case PFD

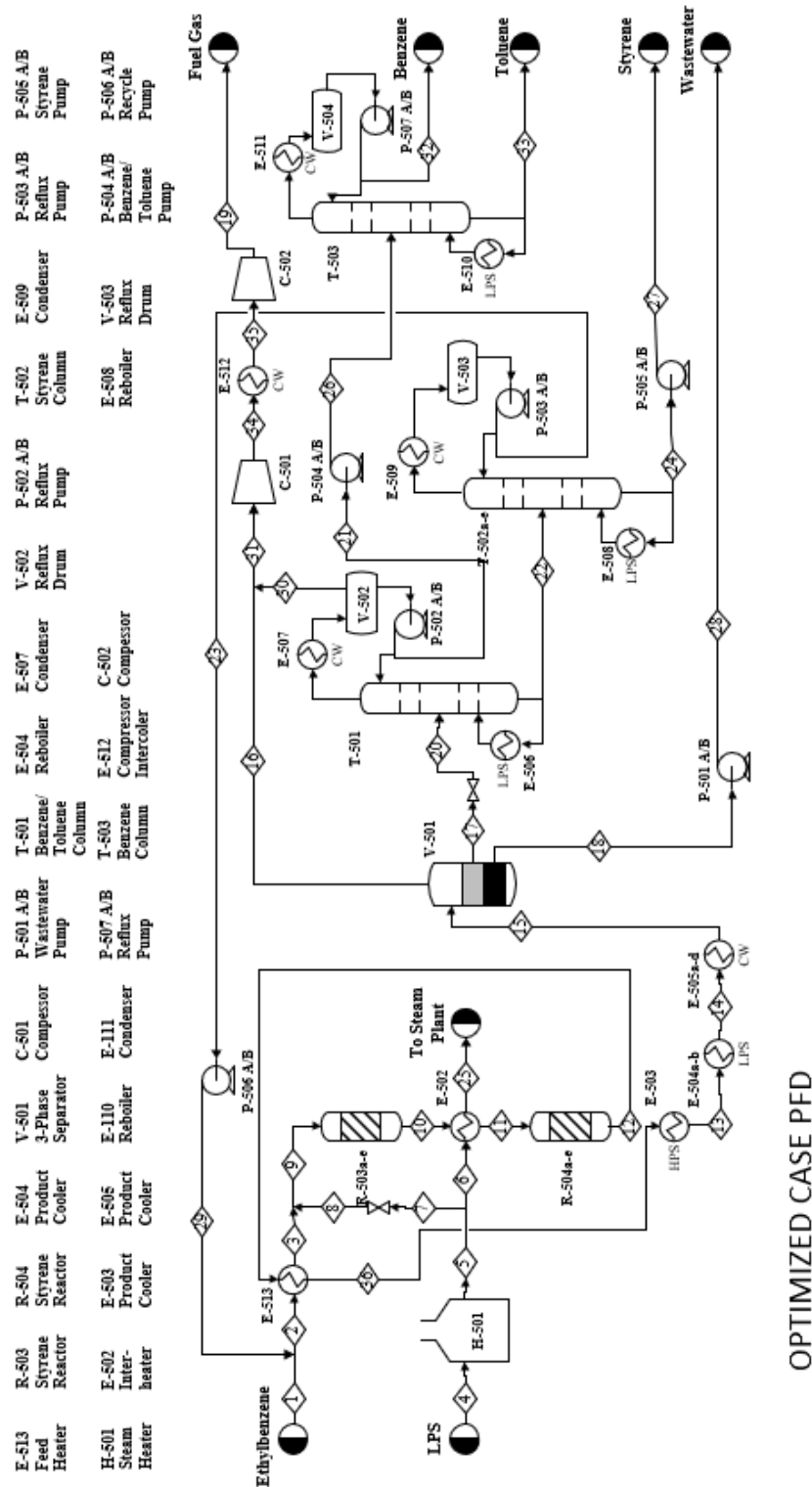


Figure 2: Base case process flow diagram as given in the problem statement

6. Optimized Case Stream Table

Stream No.	1	2	3	4	5	6	7	8	9
Temperature (°C)	136	107	225	159	800	800	800	800	525
Pressure (kPa)	203	203	188	600	565	565	565	188	188
Vapor Mole Fraction	0	0	1	1	1	1	1	1	1
Total Flow (kg/h)	19548	57071	57071	180973	180973	116368	64606	64606	121676
Total Flow (kmol/h)	185	538	538	10046	10046	6459	3586	3586	4125
Comp. Flow (kmol/h)									
Water	0	0	0	10046	10046	6459	3586	3586	3586
Ethylbenzene	181	533	533	0	0	0	0	0	533
Styrene	0	1.2	1.2	0	0	0	0	0	1.2
Hydrogen	0	0	0	0	0	0	0	0	0
Benzene	1.8	1.8	1.8	0	0	0	0	0	1.8
Toluene	1.8	2.2	2.2	0	0	0	0	0	2.2
Ethylene	0	0	0	0	0	0	0	0	0
Methane	0	0	0	0	0	0	0	0	0
Stream No.	10	11	12	13	14	15	16	17	18
Temperature (°C)	483	575	539	270	180	65	65	65	65
Pressure (kPa)	164	149	113	98	83	68	68	68	68
Vapor Mole Fraction	1	1	1	1	1	0	1	0	0
Total Flow (kg/h)	121676	121676	121676	121676	121676	121676	2928	55355	63393
Total Flow (kmol/h)	4190	4190	4268	4268	4268	4268	210	539	3519
Comp. Flow (kmol/h)									
Water	3586	3586	3586	3586	3586	3586	67	0	3519
Ethylbenzene	460	460	359	359	359	359	2.5	356	0
Styrene	63	63	121	121	121	121	0.6	121	0
Hydrogen	54	54	89	89	89	89	87	1.7	0
Benzene	6.1	6.1	25	25	25	25	1.1	24	0
Toluene	10	10	33	33	33	33	0.6	33	0
Ethylene	4.3	4.3	23	23	23	23	21	2.5	0
Methane	7.5	7.5	31	31	31	31	30	1.0	0
Stream No.	19	20	21	22	23	24	25	26	27
Temperature (°C)	157	65	50	120	91	123	700	50	123
Pressure (kPa)	240	60	40	60	25	55	555	200	200
Vapor Mole Fraction	1	0	0	0	0	0	1	0	0
Total Flow (kg/h)	221	55355	4791	50023	37523	12500	116368	4791	12500
Total Flow (kmol/h)	3469	539	55	474	353	120	6459	55	120
Comp. Flow (kmol/h)									
Water	67	0	0	0	0	0	6459	0	0
Ethylbenzene	2.6	356	3.5	353	352	0.6	0	3.5	0.6
Styrene	0.6	121	0	121	1.2	119	0	0	119
Hydrogen	89	1.7	0	0	0	0	0	0	0
Benzene	4.7	24	21	0	0	0	0	21	0
Toluene	2.4	33	31	0	0	0	0	31	0
Ethylene	23	2.5	0	0	0	0	0	0	0
Methane	31	1.0	0	0	0	0	0	0	0
Stream No.	28	29	30	31	32	33	34	35	36
Temperature (°C)	65	91	50	63	80	136	157	63	429
Pressure (kPa)	200	203	40	40	170	190	98	98	113
Vapor Mole Fraction	0	0	1	1	0	0	1	1	1
Total Flow (kg/h)	63393	37523	541	3469	20	34	221	221	121676
Total Flow (kmol/h)	3519	353	11	221	1571	3219	3469	3469	4268
Comp. Flow (kmol/h)									
Water	3519	0	0	67	0	0	67	67	3586
Ethylbenzene	0	352	0	2.6	0	3.5	3	3	359
Styrene	0	1.2	0	0.6	0	0	1	1	121
Hydrogen	0	0	1.7	89	0	0	89	89	89
Benzene	0	0	3.6	4.7	20	0.5	5	5	25
Toluene	0	0	1.8	2.4	0	30.5	2	2	33
Ethylene	0	0	2.4	23	0.1	0	23	23	23
Methane	0	0	1.0	31	0	0	31	31	31

Table 2: Optimized case stream table as calculated for ChE 451

7. Optimized Case Utility Summary Table

Utility Summary for Unit 500							
E-503		E-504		E-505		E-506	
bwf → hps		bwf → lps		cw		lps → bwf	
18588	kg/h	9486.927	kg/h	4739512	kg/h	10366.73	kg/h
E-507		E-508		E-509			
cw		lps → bwf		cw			
518690	kg/h	43652.02	kg/h	1642037	kg/h		
E-510		E-511		E-512			
cw		lps → bwf		cw			
53053	kg/h	1060.334	kg/h	19547.29	kg/h		

8. Optimized Case Equipment Summary Table

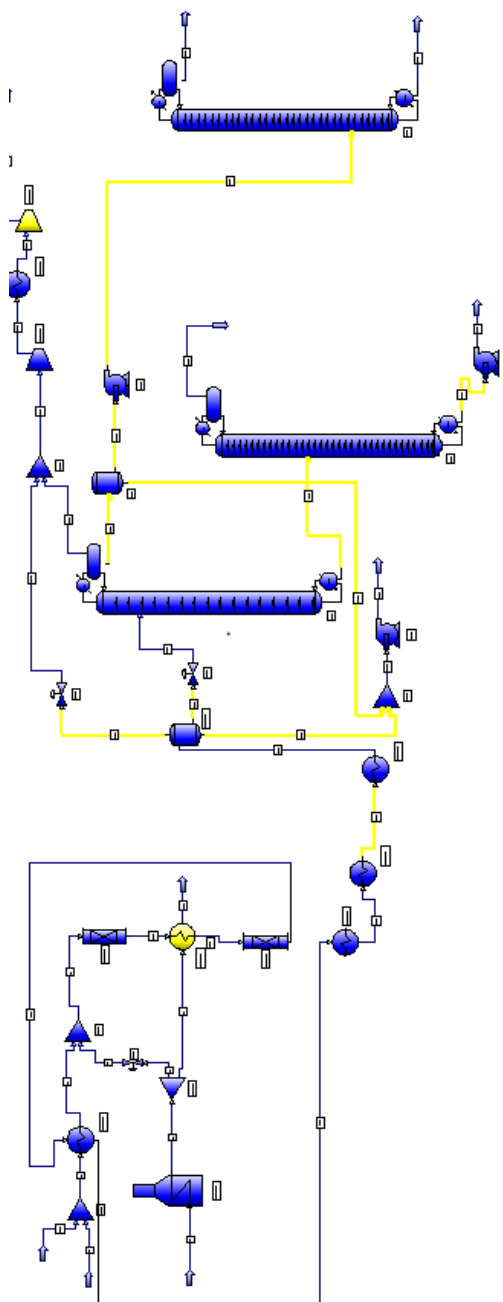
Heat Exchangers							
E-501				E-502			
A =	339.5187	m ²		A =	162.6254	m ²	
1-2 exchanger, fixed tube sheet, carbon steel				1-2 exchanger, floating head, 316 SS			
Process side pressure drop = 15 kPa				Process side pressure drop = 15 kPa			
E-503				E-504a-b			
A =	1338.808	m ²		A =	474.3989	m ²	
1-2 exchanger, fixed tube sheet, 316 SS				1-2 exchanger, fixed tube sheet, carbon steel			
Process side pressure drop = 15 kPa				Process side pressure drop = 15 kPa			
E-505a-d				E-506			
A =	419.1813	m ²		A =	177.7396	m ²	
1-2 exchanger, fixed tube sheet, 316 SS				1-2 exchanger, fixed tube sheet, 316 SS			
Process side pressure drop = 15 kPa							
E-507				E-508			
A =	517.4387	m ²		A =	499.8216	m ²	
1-2 exchanger, floating head, carbon steel				1-2 exchanger, fixed tube sheet, 316 SS			
E-509							
A =	471.7084	m ²					
1-2 exchanger, floating head, carbon steel							

Pumps							
P-501 A/B				P-502 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	2.263131	kW		Actual power =	3.450626	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-503 A/B				P-504 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	23.19948	kW		Actual power =	0.643176	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-505 A/B				P-506 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	0.742584	kW		Actual power =	1.504448	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
Fired Heater							
H-301							
Fired heater - refractory lined, stainless steel tubes							
Required heat load =	123309.8	MJ/h					
Design (maximum) heat load =	164.413	GJ/h					
Thermal Efficiency =	0.75						

Pumps							
P-501 A/B				P-502 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	2.263131	kW		Actual power =	3.450626	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-503 A/B				P-504 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	23.19948	kW		Actual power =	0.643176	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
P-505 A/B				P-506 A/B			
Carbon Steel - centrifugal				Carbon steel - centrifugal			
Actual power =	0.742584	kW		Actual power =	1.504448	kW	
Efficiency =	0.75			Efficiency =	0.75		
Electric Drive				Electric Drive			
Fired Heater							
H-301							
Fired heater - refractory lined, stainless steel tubes							
Required heat load =	123309.8	MJ/h					
Design (maximum) heat load =	164.413	GJ/h					
Thermal Efficiency =	0.75						

Compressors and Drives			
C-501		D-401 A/B	
Carbon steel		Electric/explosion proof	
W =	538.1611 kW	W =	717.5481 kW
Adiabatic Efficiency =	0.75	Efficiency =	0.98

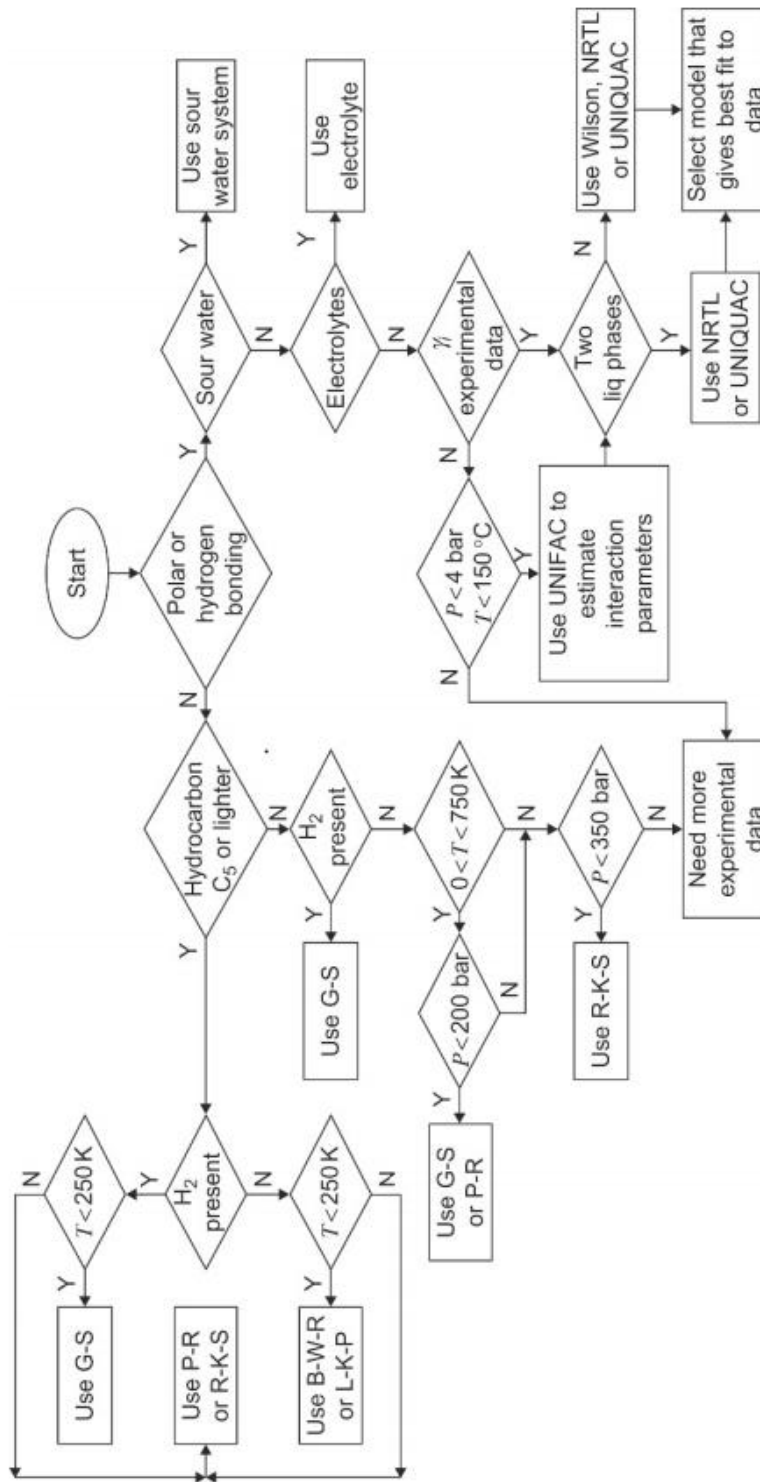
9. Optimized Case Pro/II



10. Optimized Case Income/Cash Flow Statement

End of Year	Income and Cash Flow Statement (Sylvane Case Key Spring 2018)														
	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032
	-2	-1	0	1	2	3	4	5	6	7	8	9	10	11	12
Depreciation	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000	5,000,000
Land (BV)															
Building															
Bldg BV															
Machines															
Mach BV															
Tools															
Taxable Income															
Income Taxes															
Net Income															
Operating Activities															
Net Income															
Depreciation															
Investment Activities															
Land															
Buildings															
Machines (FCI or Cap ex buildings and land)															
Tools															
Gain/Tax															
Working Capital															
Net Cash Flow															
Cumulative Cash Flow															
PV (SIU) @ 12%															
Cumul/Discounted CF															
NPV (12%)	30,566,898	AE (12%)	4,334,622.41												
MARR	12%	DCFPR	16%												

11. Thermodynamic Flowsheet



Appendix C- Optimization Materials and Steps

1. Sensitivity Graph

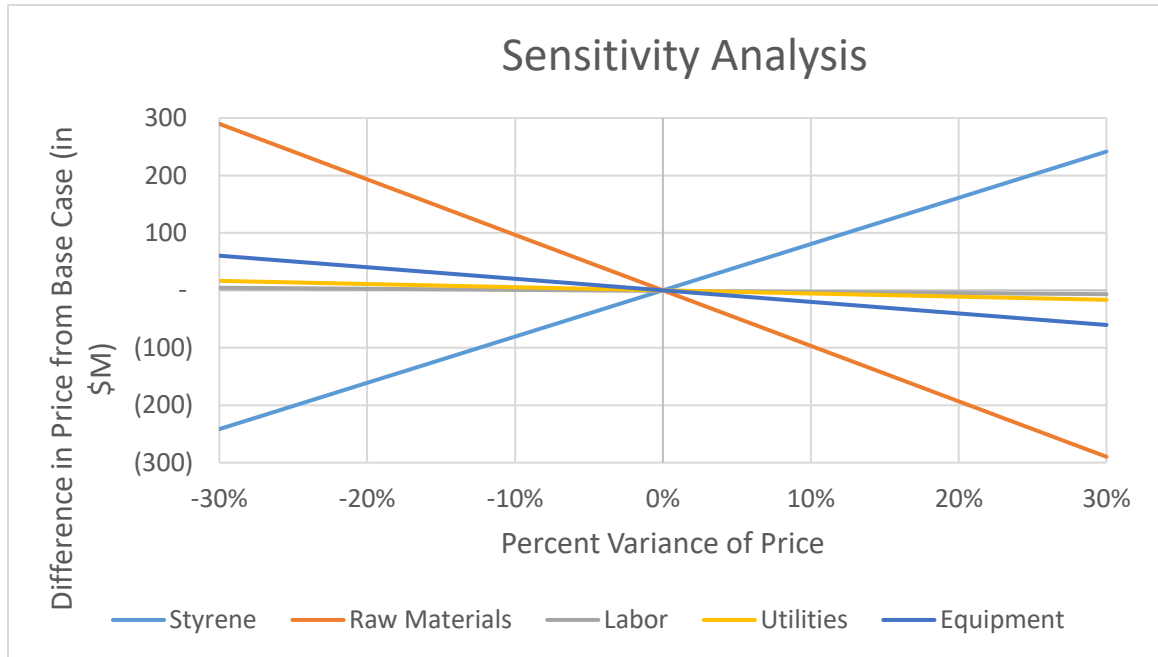


Figure 3: Results from sensitivity analysis completed on the base case styrene process

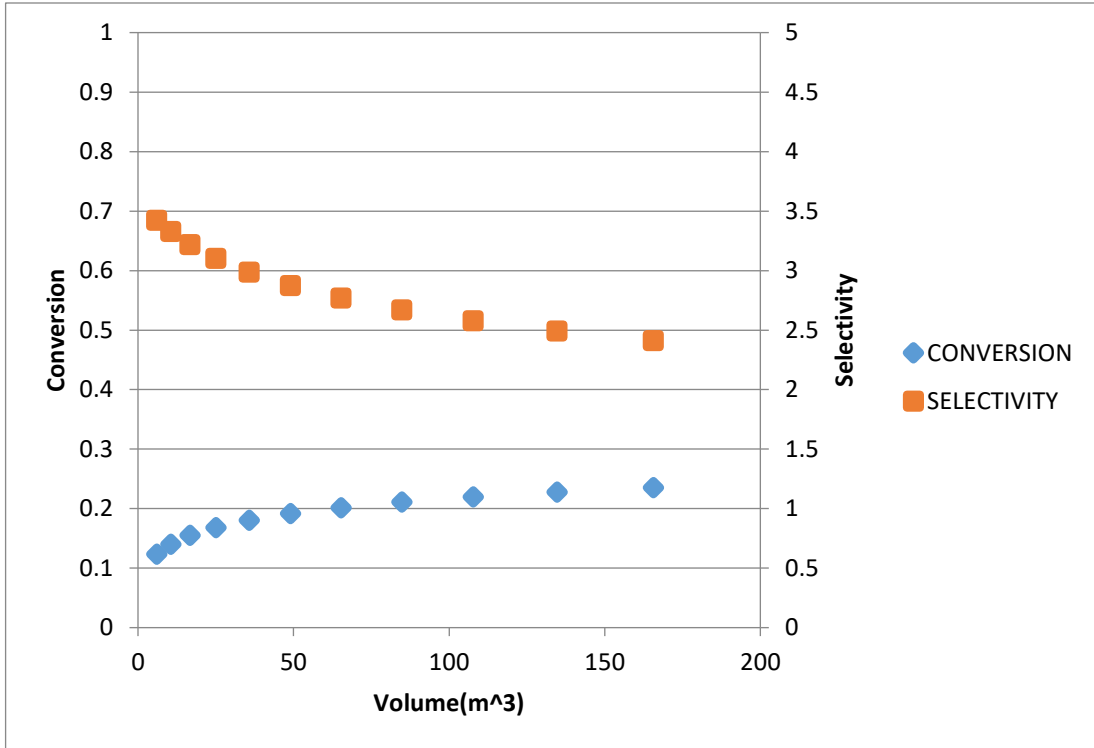
2. Economic Comparison (Reactor Type)

NPV Contribution	Isothermal	Adiabatic	Difference
Raw Materials	-\$1178 M	-\$1008 M	\$170 M
Utilities	-\$69 M	-\$66 M	\$3 M
FCI	-\$137 M	-\$190 M	-\$53 M
NPV	-\$320 M	-\$264 M	\$56 M

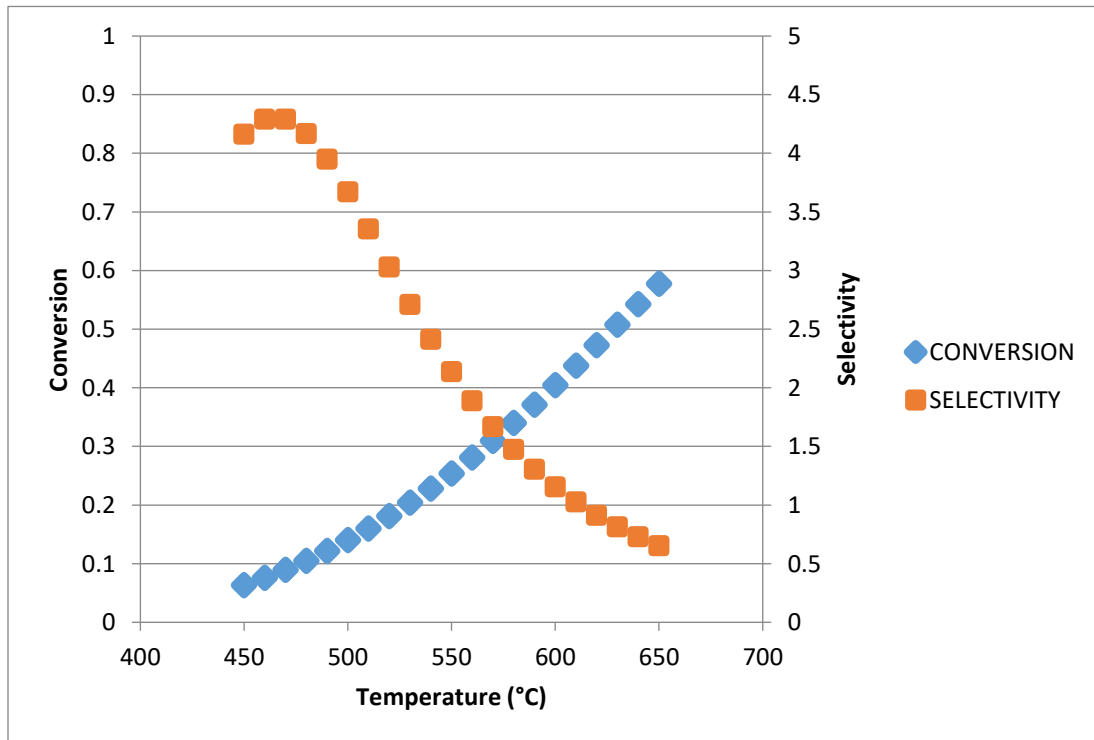
3. Economic Comparison (Reactor Conditions)

NPV Contribution	Adiabatic	Adiabatic with Changes	Difference
Raw Materials	-\$1008 M	-\$874 M	\$134 M
Utilities	-\$66 M	-\$74 M	-\$8 M
FCI	-\$190 M	-\$226 M	-\$36 M
NPV	-\$264 M	-\$204 M	\$60 M

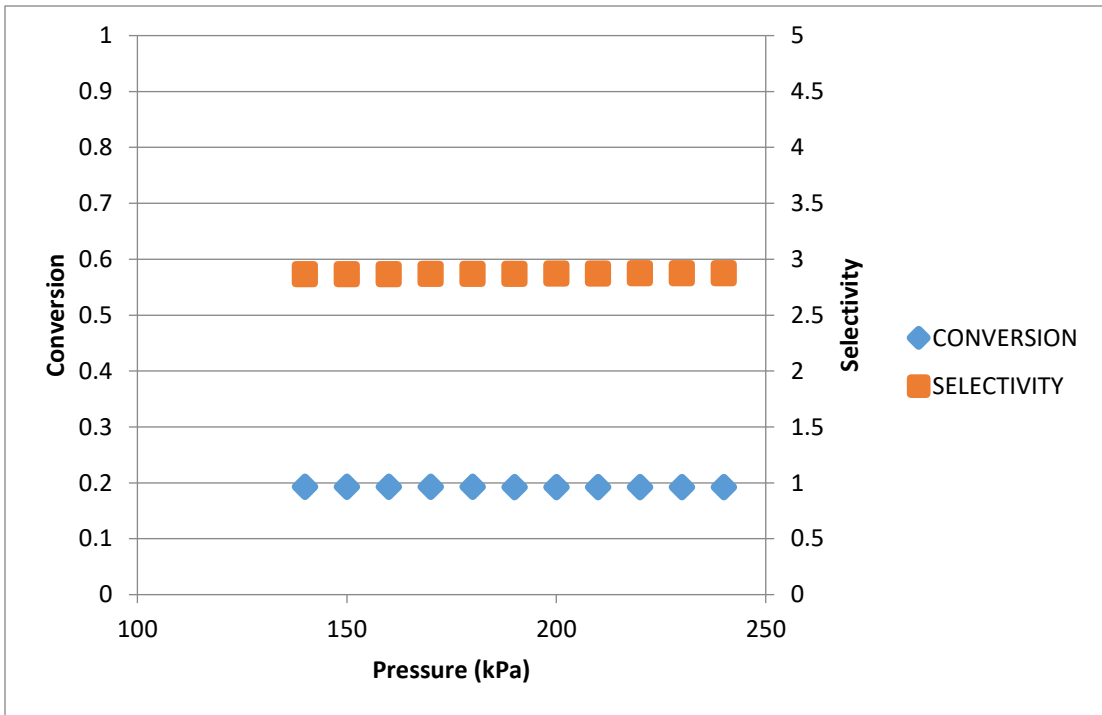
4. Conversion vs. Selectivity (Volume of R-503)



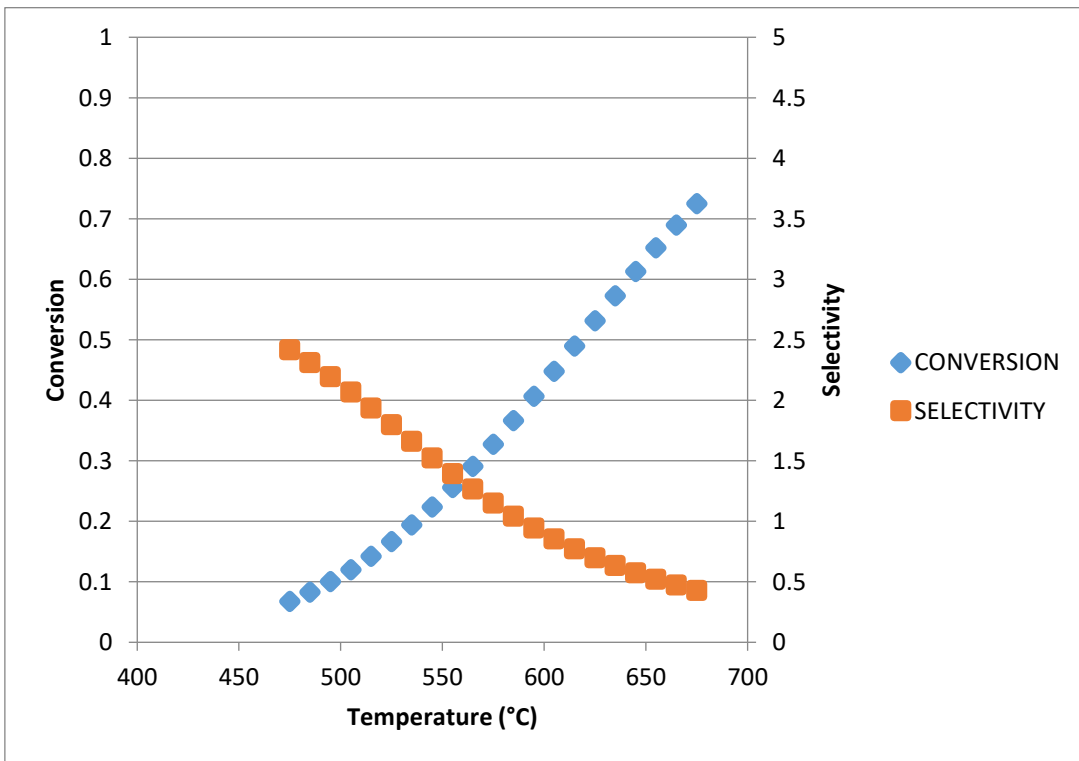
5. Conversion vs. Selectivity (Temperature of R-503)



6. Conversion vs. Selectivity (Pressure of R-503)



7. Conversion vs. Selectivity (Temperature of R-503)



8. Economic Comparison (Materials of Construction)

NPV Contribution	No Material Change	With Material Changes	Difference
Raw Materials	-\$875 M	-\$875 M	-
Utilities	-\$74 M	-\$74 M	-
FCI	-\$226 M	-\$114 M	\$112 M
NPV	-\$204 M	-\$39 M	\$165 M

9. Economic Comparison (Heat Integration)

NPV Contribution	Without HI	With HI	Difference
Utilities	-\$74 M	-\$72 M	\$2 M
FCI	-\$114 M	-\$114 M	\$0.3 M
NPV	\$16 M	\$20 M	\$4.1 M

10. Economic Comparison (Base Case vs. Optimized Case)

	Base Case	Optimized Case
NPV	-\$320 M	\$31 M
DCFROR	N/A	16%
AE	-\$52 M	\$5 M

Appendix D- Miscellaneous Information

1. Rate Laws

$$r_1 = 6.2 \exp\left(\frac{-90,981}{RT}\right) P_{cb}$$

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

$$r_3 = 2.71 \times 10^7 \exp\left(\frac{-207,989}{RT}\right) P_{cb}$$

$$r_4 = 6.45 \times 10^{-4} \exp\left(\frac{-91,515}{RT}\right) P_{cb} P_{H_2}$$

where p_i is the partial pressure of component i in Pa, T is the temperature in K, the activation energy is in J/mol, and the rate is in mole/(m³ catalyst* second).

2. Notes About November 2018 Presentation Deficiencies

Our engineering team addressed several deficiencies noted by the presentation panel in this report. First, we fixed errors in the PFDs, which included changing the names of the adiabatic reactors to R-503 and R-504, aligning the input and output streams on the far left and far right sides of the page, and ensuring that stream 19 remained the fuel gas stream exiting the plant. The panel also noted that the temperature of the process is above the flash point of each component. The finished process safety section in the paper includes this. Lastly, the panel noted a lack of sources for why the team decided to use stainless steel clad as the material for towers T-501 and T-502; therefore, after further research, the team selected carbon steel as the tower material and documented the source used in the works cited section.

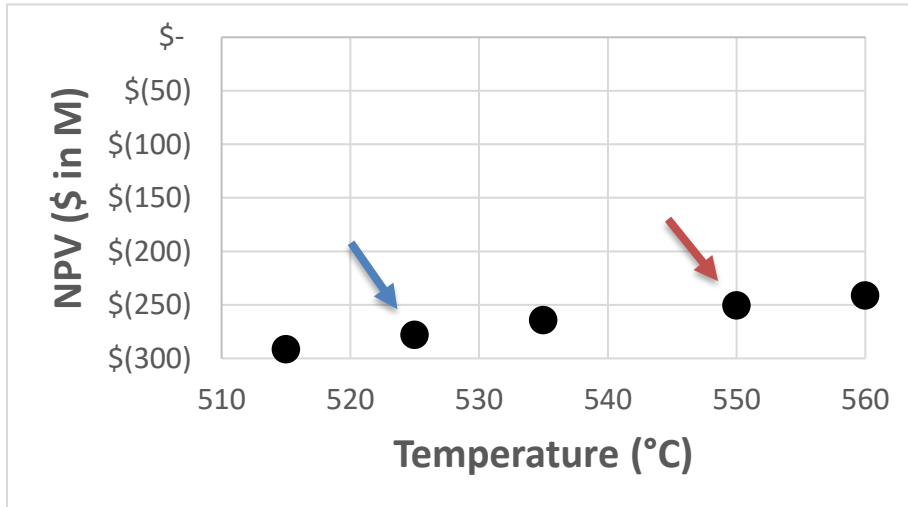
We also corrected calculation errors. For the presentation, we made graphs showing the change in selectivity and conversion as temperature and pressure changed in

the reactor section; however, we used the incorrect definition for selectivity. Originally, the engineering team defined it as the yield of styrene divided by the total amount of all side products (benzene and toluene) and by products (hydrogen, ethylene, and methane). Now, the definition is the yield of styrene divided by only the side product total. In addition, a calculation issue in Excel occurred when the team originally added tower T-503. The additional separation caused an increase in the raw materials cost for the total process when solving the mass balances, which did not make sense as it should only be separating the pre-existing stream. We corrected this by using a separate tab for the T-503 calculation.

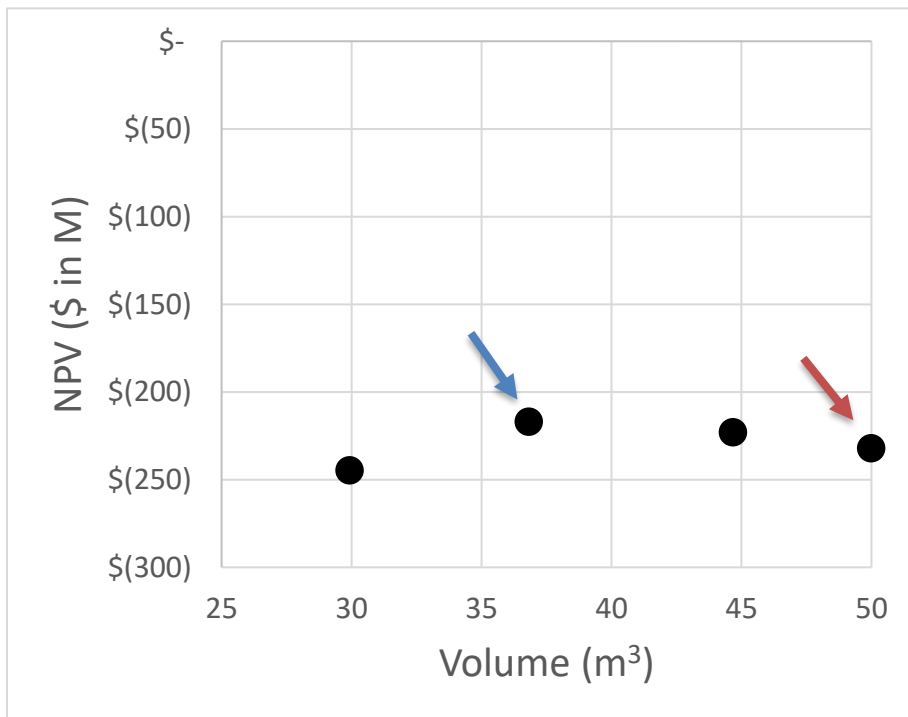
Lastly, the most significant deficiency noted was that our graphs and tables were not effective. Our original tables put prices per year, one-time costs, and NPV in one place, and we denoted the significance of each adjustment in the process with percent changes. We corrected all tables in Appendix C so they display NPV contributions (the panel asked us to either put all the values in terms of NPV or equivalent annual operating costs- EAOs.) We relocated these figures into the Appendix section to make them accessible to the reader but also to keep them separate so that they do not become a distraction (the panel mentioned this during the presentation.) In addition, we made the graphs shown below for the presentation; however, the NPV values are now incorrect as we found that we did not remove the utility cost for the isothermal reactors once we changed them to adiabatic. However, despite this mistake, the trends observed in the graphs did not change and this still influenced the team's design choices. If given more time, the team would correct these to properly reflect the accurate NPV.

3. R-503: Change in Temperature vs. NPV

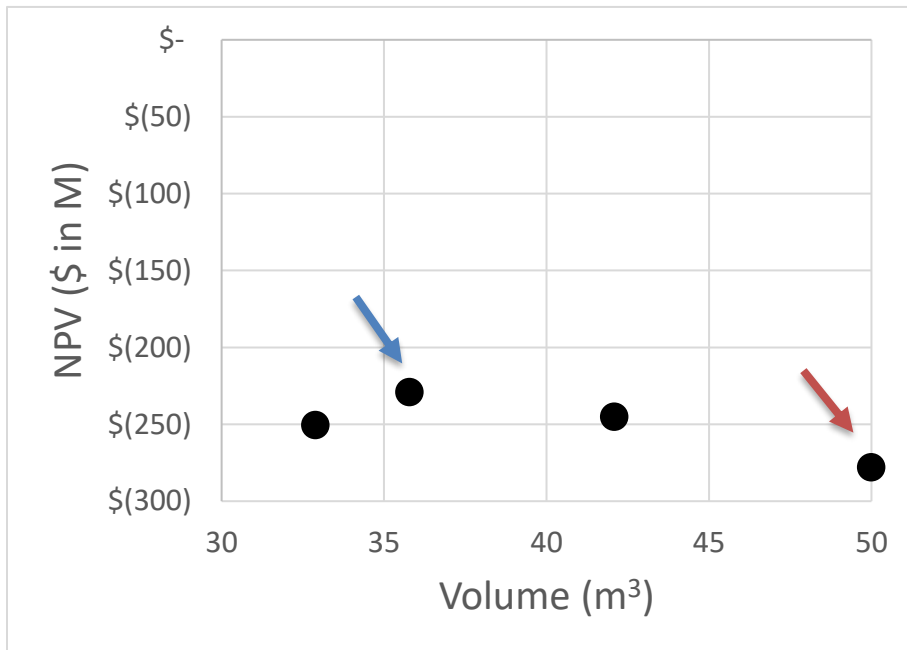
***Red indicates Base Case/Blue indicates Change**



4. R-503: Change in Volume vs. NPV



5. R-504: Change in Volume vs. NPV



Appendix E- Fluidized Bed Reactor Pro-II Simulation

Stream Name	Stream Description	Phase	S4
Temperature		C	549.9880
Pressure		KPA	133.5098
Enthalpy		M*KJ/HR	294.8993
Molecular Weight			27.0229
Mole Fraction Vapor			1.0000
Mole Fraction Liquid			0.0000
Rate		KG-MOL/HR	4012.000
Fluid Rates		KG-MOL/HR	
EBENZENE			231.6935
H2O			3486.8000
STYRENE			90.7019
H2			65.1952
BENZENE			24.1978
TOLUENE			27.4067
ETHYLENE			21.6978
METHANE			24.3067



Figure 3: Converged Pro-II flowsheet for the fluidized bed reactor in the base case styrene process (and associated component flowrates in the product stream)

Total	4018.2	kmol/hr
Water	3467	kmol/hr
Ethylbenzene	282	kmol/hr
Styrene	95	kmol/hr
Hydrogen	66.0	kmol/hr
Benzene	26.4	kmol/hr
Toluene	30.6	kmol/hr
Ethylene	23.9	kmol/hr
Methane	27.5	kmol/hr

Table 3: Product stream from the fluidized bed reactor in the base case styrene process (as calculated in the Excel model). When compared to the values calculated by Pro-II, the Excel model appears to be a good approximation.

References

- [1] R. Turton, R. C. Bailie, W. B. Whiting and J. A. Shaeiwitz, *Analysis, Synthesis and Design of Chemical Processes*, 3rd Edition, Prentice Hall, 2009.
- [2] R. Cocco, S. B. R. Karri and T. Knowlton, "Introduction to Fluidization," *CEP Magazine*, November 2014.
- [3] "Hydrogen Embrittlement," [Online]. Available: www.nace.org/Corrosion-Central/Corrosion-101/Hydrogen-Embrittlement/.