2015

A Look Into Process Optimization

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Recommended Citation

Lambert, Joshua Hunter, "A Look Into Process Optimization" (2015). *Honors Theses*. 489.
https://egrove.olemiss.edu/hon_thesis/489

A LOOK INTO PROCESS OPTIMIZATION

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

Oxford
May 2015

Approved by:

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THIS THESIS IS DEDICATED TO MY FATHER.

ACKNOWLEDGMENT

I would like to thank Dr. Adam Smith for all the guidance he has given me over the past three years of my academic career. He has always pushed me in the right direction and always challenged me to do my best. I would also like to thank Alec Mattei for being my group partner throughout the optimization of the Ethylbenzene process.

ABSTRACT

HUNTER LAMBERT: A Look Into Process Optimization

(Under the direction of Adam Smith and the help of Alec Mattei)

The goal for this paper is to inform the reader on the optimization process in chemical engineering design. The reader will gain knowledge about the step-by-step process as well as terminology of the optimization journey. Optimization takes a great amount of work, and it can be a daunting task if one gets caught up in the minute details. However, I will show that looking at the big picture will drastically ease the process and make optimizing much simpler.

A base case will first be presented. The base case should be modeled using a process simulator, and then an economic analysis should be performed. The objective function of the base case will then be compared to future optimizations. Next, changes may be presented to the case. Changes must then be simulated and analyzed. Finally, different processes throughout the facility must be optimized to present even more cases. The case that optimizes the objective function is the case that will be chosen as the best.

In the final section of the paper, I will present an ethylbenzene plant optimization that was performed earlier. There were decisions that were made based on the performance of the process. I chose to buy a lower grade of benzene feed and used a new catalyst that was offered. Also, I decided to operate the reactor train at high temperature and pressure due to the high benzene conversion. These are my recommendations. The net present value (NPV) of the process is increased by approximately $50 million.

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Introduction

When it is necessary to improve a plant, piece of equipment, or a design, going through the steps of process optimization proves to be a great method to follow. This paper will highlight the key points of optimization. Important terms, different methods, and key decision variables will be pointed out. In the last section, a specific case of process optimization will be explained. My group partner, Alec Mattei, and I were presented with a base case of an ethylbenzene plant. We then simulated this base case in the computer simulator Pro/II. After an economic analysis of the base case, we calculated a net present value (NPV) of -$10.4 million. After being presented with two suggestions and making our own changes to the process, we were able to raise the NPV to $39 million. This increase of $50 million over a 14-year period shows that process optimization is a worthwhile venture.

General Optimization

Optimization can be described as the process of improving an existing situation, device, or a system such as a chemical process. The process of optimization can be a great amount of work, but there are certain steps that should be taken to shorten the process. First, an optimization problem must be presented. A base case will often be given that results can be compared to, but this is not the case all of the time. Sometimes the user will have to first simulate the process. Next, after a basis has been completed, the value of potential improvement must be quantified. It should be clear where there is room for improvement in the process. Then, the constraints of the process must be accounted for and any type of barriers or bottlenecks must be identified. This will be explained in more detail below. Changes should now be made to the process to try and optimize the process. Results of these changes should be analyzed to see which changes should be made. Finally, evaluate the results to see if the user feels like an adequate process optimization has been performed. This is process optimization summed up into a very basic guide. Now, I will give into a more detailed description of what process optimization is about.

Terminology

To understand process optimization, the terminology must first be understood. There is a vast amount of terms, but I will sum up the most important ones in this section. The first term that should be known is decision variables, or also known as design variables. These are the independent variables that engineers have some control over. These can be things such as pressure of a reactor, or the pressure drop across a distillation column. A very important part of process optimization is the objective function. This is, ultimately, the mathematical function that will determine how well the optimization was performed. The objective function is a function of the decision variables that are manipulated earlier in the process. The goal of optimization is to maximize (or minimize in some scenarios) the objective function. If it is a profit, the objective function should try and be maximized. If it is a cost, then the objective function should be minimized. On occasion, there may be more than one objective function in a given problem.

As mentioned earlier, a given process usually has a number of constraints on it. Constraints are limitations that must be accounted for when changing the decision variables. Equality constraints are a given value that is exact. An example of this is a set temperature or pressure a reactor must be set to operate. Inequality constraints are when decision variables must operate above or below a certain point. Examples of these are when a certain pressure or temperature cannot be exceeded in a column, or when a reaction must operate below a certain temperature to prevent chemical degradation. The dimensionality of a project is the number of truly independent variables in a process. When an equality constraint is given, then the dimensionality of the process is reduced. By reducing the dimensionality of the project, the project becomes easier to optimize.

Types of Optimization

The word optimum can be defined as the greatest degree or best result obtained under specific conditions. Optimization can then be broken down into two separate types. There is a global optimum, which is the point that the objective function is the best it can be under the given conditions. In real world scenarios, the global optimum is never reached for a whole process. The next type of optimum is a local optimum. This is when a point is reached where small changes in either direction will not maximize (or minimize) the objective function any more. There are also different classes of optimization that can be analyzed. If all the decision variables correlate with the objective function in a linear manner, then the optimization is linear. These are usually easier than other optimizations because there is an algorithm that can solve the function. The other class of optimization is non-linear. If it is a second order relationship, then it is a quadratic programing optimization.

I mentioned earlier that optimization could seem like an intense, complex process that involves endless amount of work. While optimization can be daunting, it is a nice brainstorming activity that can be very rewarding. When brainstorming ideas, it must be remembered that we must apply real world strategies to our process. Having an extremely tall distillation column may optimize a process, but this may exceed safety regulations. Taking into account real world scenarios can shorten the amount of work it takes to optimize a process. Another thing to consider when optimizing a process is to consider if a local optimum can be improved upon. While a local optimum is ok in certain scenarios, it is beneficial to expand the search to see if there is a greater optimum that can be found.

Strategies for Optimization

There are certain strategies for attacking process optimization. As I mentioned earlier, a global optimum will likely not be found for a whole process because this would take a great amount of time for a whole process with a great amount of minuscule changes. The first strategy to start optimization is to look at the big picture of the project, then dive into the smaller details. This strategy is called top-down. The other type of strategy that can be implemented in optimization is the bottom-up strategy. Unlike top-down, this strategy uses a detailed study of incremental changes to see how the big picture is affected. When a case is first presented, it is beneficial to take a top-down approach first. However, when a roadblock is reached, it can be helpful to start looking at minor details and see how they affect the process. It is best to use both strategies accordingly when performing optimization.

The sensitivity of the optimum can be described as the rate at which the objective function changes with changes in one of the decision variables. It would not be wise to base the whole process on a decision variable that is very sensitive to change because this means that there is not any stability in the findings. It would be better to base your results on changes that are not very sensitive because then the project is beneficial over wide ranges and can overcome minor upsets in the process. All of this can be represented visually with a sensitivity analysis.

The base case in an optimization project is the starting point. It can be anything from an idea to a detailed design. Choosing a base case usually incorporates the best available case that is available at the beginning of the optimization process. When looking at the level of detail in the base case, it is important to be able to calculate an objective function from the base case. If this is not possible from the base case, then it is obvious that there are more details needed. The scope should also match the scope of the optimization that is going to be performed.

There are a number of questions that need to be asked when performing optimization. Some examples of these are: Can unwanted by-products be eliminated?

Can any equipment be eliminated? Can anything be rearranged to make the process better? To what extent can heat integration be improved? To answer these questions, we should address them approximately in the order listed above. To eliminate unwanted by-products, the conversion of reactants and selectivity of the reactions should be maximized. Both eliminating and rearranging equipment can lead to substantial progress in case studies. Usually, every piece of equipment that is included in a PFD is there for a reason and not redundant. However, sometimes equipment can be eliminated when the inlet conditions are changed in the process. Things to keep in mind when arranging equipment is to think of which scenario takes less work to achieve the goal. An example of this would be pumping a liquid instead of compressing a gas. It would be beneficial to put a pump before a vaporizer instead of a compressor after a vaporizer. Lastly, heat integration should be used within a plant whenever it is possible. A plant can save a great amount of money by utilizing any type of heat streams that can be recycled within the facility. All of the questions outlined in this paragraph are keys to successfully optimizing a plant.

Key Decision Variables

The choice of key decision variables when optimizing is very important because it can limit the amount of work and time that will be put into the project. Outlined in this section are lists of common decision variables that can be investigated to optimize a plant. The first are the reactor(s) operating conditions. Examples of things that can be changed in reactors are the operating temperature, pressure, and concentration of reactants. Case studies and calculations can be performed to optimize the objective function in a process by varying these factors. The next variable that should be looked at is the single pass conversion in the reactor(s). Maximizing this will improve the performance of the overall process. It is important that any unused reactants are recovered in the process. The raw materials in a process are often the greatest cost that a plant will encounter. This is why it is vital to make sure that the greatest amount is used or recovered in a process. Other variables to consider are the purge ratios of inert products, reflux ratio in columns, and the flow of mass separating agents in absorbers, strippers, etc. Investigating all of these options can ultimately optimize the objective function. These key decision variables are very important to be investigated, however, they are not the only ones that should be looked at. There are numerous variables that can be changed in the plant. Remember that every time a change is made it is important to update the objective function to see if change is favorable.

This sums up what the process of optimization entails. Optimization is an intricate process, but there are certain steps that can be taken to shorten the amount of work needed to perform optimization. It is always important to remember to keep the main focus of the project on the objective function. It can be easy to get caught up in the details of the project. However, stay on track to try and present an optimized case that is not very sensitive to changes in the system.

Ethylbenzene Case Optimization

A specific example of process optimization will be outlined in this section of the paper. If more in-depth info is wanted relating to the process about to be described, then it can be found in the Appendix. My group partner, Alec Mattei, and I were presented with a base case of an ethylbenzene plant. We then simulated this base case in Pro/II. After an economic analysis of the base case, we calculated an NPV of -$10.4 million.

Next, we were presented with two changes that could be made to the facility. The first change was to use a new type of catalyst, and the second change was to use a lower grade of benzene feed at a cheaper price. This left us with four different options that could be made. We could use neither of the changes, either of them, or both of them. We simulated the changes, and we investigated how they affected our objective function (net present value in this case). The option that maximized out NPV was chosen. This happened to be making both changes. This brought the NPV to $31.9 million. Now, we had full range to play with any variables so long as we were within constraints and that we met the given specifications. The specifications that we had to meet were to produce 80,000 tonne/yr of 99.8 mol% ethylbenzene that will later be consumed by an on-site styrene plant. The composition of our product ethylbenzene stream must not contain more than two parts per million (ppm) of diethylbenzene. A process concept diagram of the main reaction is presented below in Figure 1. Benzene will be reacted with ethylene to produce ethylbenzene. This is the basis of the ethylbenzene facility.

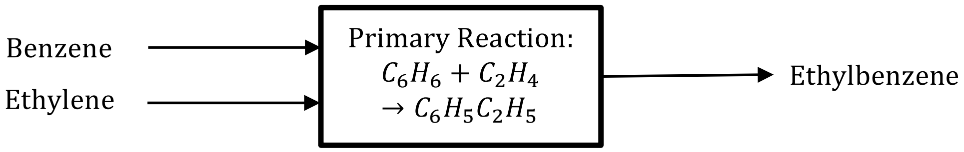

Figure 1. Process Concept Diagram of Ethylbenzene Facility

Throughout the optimization of the process, we made many assumptions in order to simplify the analysis of our process. We assumed that the land costs were negligible, and the design for the process would be for a new, grass-roots facility. We also assumed that the taxation rates would be 45% per year for the duration of the project. The construction period is two years with a distribution of 60% at the end of year one and 40% at the end of year two. The project would last for twelve years after the construction period ended which would occur at the beginning of year three. The capital investment will depreciate under the MACRS 7 year category. After the twelve years that the project lasts, we assumed that the salvage value is 10% of the fixed capital investment. We also assumed that the labor costs would increase at a rate of 3% per year. In order to calculate the net present value of the plant, we assumed a minimum acceptable rate of return (MARR) of 12%. We assumed that the costs for our raw materials, products, and utilities would stay constant for the duration of the project.

In our ethylbenzene facility, there were three main sections; a reactor feed section, reactor section, and separation section. This can be shown in the block flow diagram below in Figure 2.

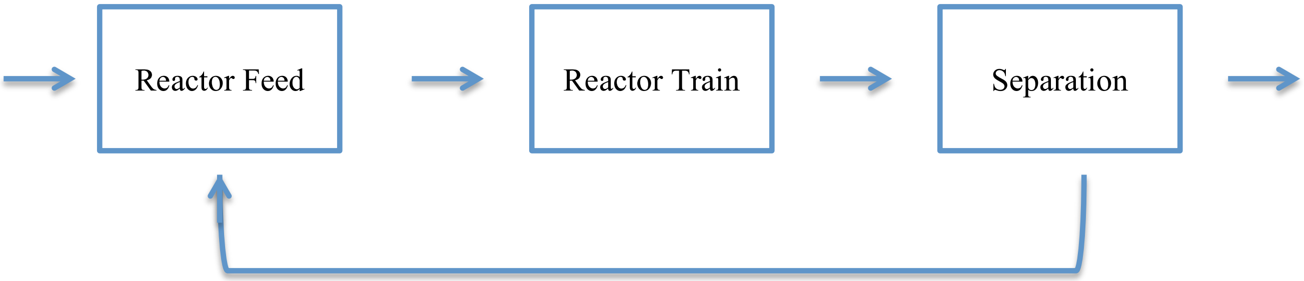

Figure 2. Ethylbenzene Block Flow Diagram

In our optimization, most of the improvement of the project came in the reactor train. This is because we were able to convert more of our benzene feed into ethylbenzene, and we were able to increase our selectivity of ethylbenzene over diethylbenzene. This is why I am going to focus on describing the reactor train optimization in more detail. However, it should be known that other parts of the plant were optimized, such as the flash vaporization tank and distillation column, to maximize the objective function (NPV).

In our reactor train, we were operating with three areas of concern. We had a high temperature, high pressure, and a non-stoichiometric feed. We were not able to change our non-stoichiometric feed because the catalyst manufacturer told us to keep an 8:1 ratio to ensure that no tri- or higher ethylbenzenes were produced. This left us with two areas of concern to look at, temperature and pressure. The temperature range was varied from 200°C to 435°C. The changes we investigated were the conversion of benzene after a single pass through the entire reactor train, and the selectivity of ethylbenzene over diethylbenzene. We stopped at 435°C because if we went any higher, then our effluent would be greater that 500°C. 500°C was our max operating temperature because the catalyst manufacturer gave us this guideline to prevent catalyst poisoning. The result of this case study can be seen in Figure 3 on the next page.

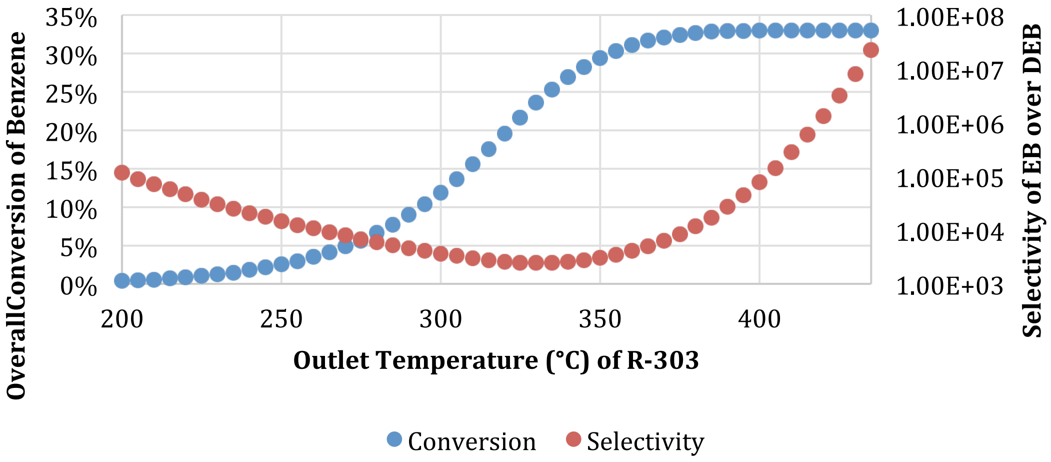

Figure 3. Overall Conversion of Benzene and Selectivity of Benzene/Diethylbenzene vs. Temperature

It can be seen in Figure 3, that as we increase the temperature, both the conversion and selectivity increase. It would appear that this would be the route to take. However, this would make us have to build our reactors out of special material. We investigated the economic factors of operating at high temperatures with special material versus operating at lower temperature and found that it was beneficial to operate the reactors at high temperature.

Next, we decided to investigate the effect that pressure had on the reactor train. Heuristics tell us that if we do not operate less than 1000 kPa that we will have to build thicker walled equipment. We ran a case study comparing the selectivity of EB to DEB and the conversion of benzene from 1000 kPa to 2000 kPa. The chart from this case study is presented in Figure 4.

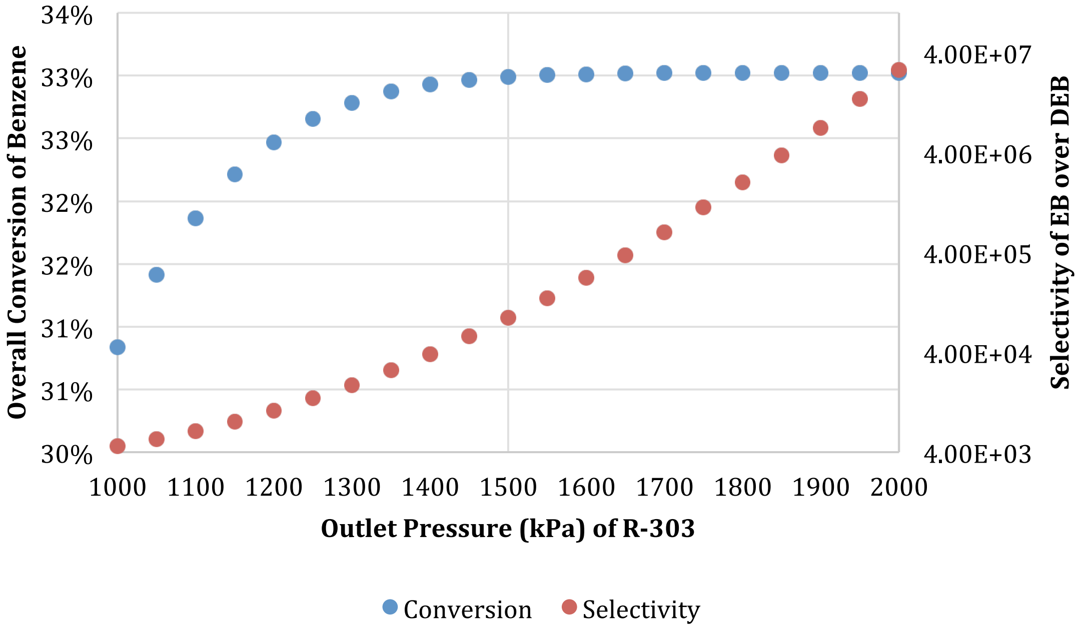

Figure 4. Overall Conversion of Benzene and Selectivity of Benzene/Diethylbenzene vs. Pressure

Figure 4 shows us that our conversion does not vary much with pressure; however, there is a decrease in the selectivity of EB when the pressure is decreased in the reactor train. Our reactor lengths would have to be nearly tripled to meet our specification of 80,000 tonne/year of EB. It would be more economical to run the reactors at high temperature rather than having extremely large reactors.

After making the decisions to operate at high temperature and pressure, there was practically no DEB contained in the reactor train effluent stream. This would allow us to eliminate a distillation column, plug flow reactor, and a recycle stream. The NPV of the process increased to approximately $32.4 million and we decide to progress our optimizations with this change due to the increased NPV. Now that we have our reactor temperatures and pressures defined, we wanted to explore the option of putting in a fourth reactor in the reactor train. Theoretically, we believed that adding in another reactor to the reactor train would in turn increase our conversion of benzene to EB and the selectivity of EB. With only three reactors in the reactor train, we had selectivity of EB to DEB of 3.5×10^7 and a conversion of benzene of 33%. When we put in a fourth reactor, our selectivity decreased to 7.2×10^5 but our conversion increased to 40%. Even though our selectivity decreased, practically no DEB was being produced. Due to the conversion increasing by about 7 %, we were able to decrease the amount of raw materials that was needed for our process because we were losing less benzene in the fuel gas. Putting in a fourth reactor meant that we would also have to put in another heat exchanger, thus increasing our capital costs. However, our NPV was still increased to $36.8 million because we were saving money in raw materials. As it shown in sensitivity analysis in Figure 5 below, the NPV is very sensitive to any change in the raw materials.

This means that decreasing the amount of raw materials we have to buy will greatly increase our NPV.

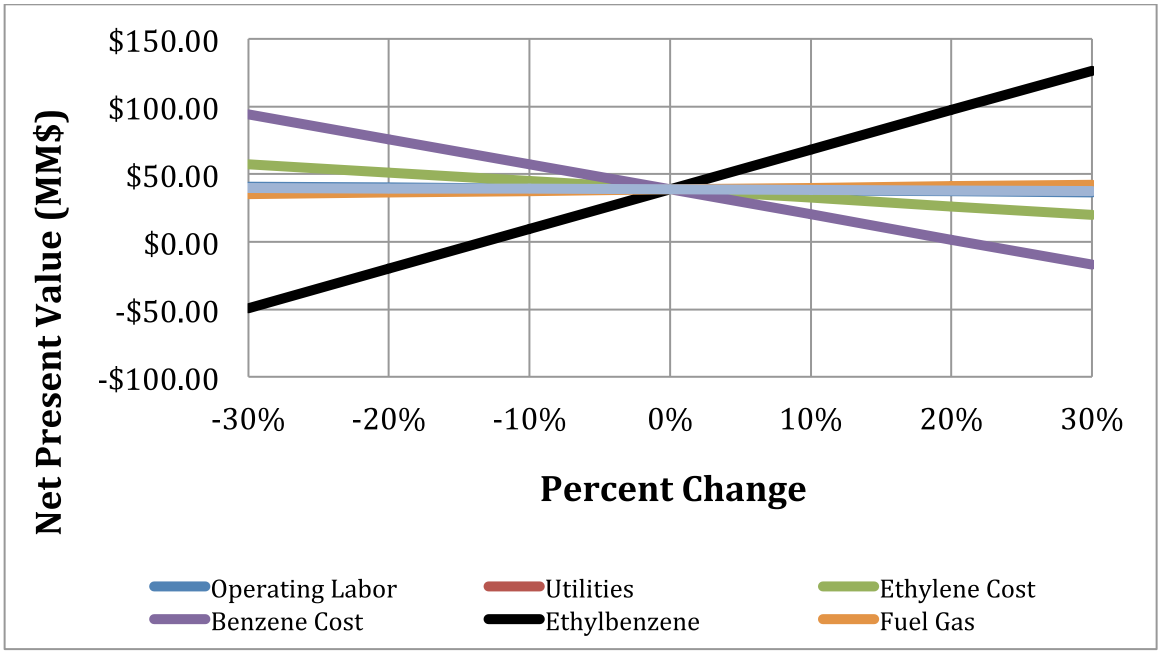

Figure 5. Sensitivity Analysis for the Optimized Process

In order to minimize the capital costs for our reactors and catalyst cost, we determined that our optimum lengths in Pro/II would be 4.95m, 5.36m, 5.84m, and 6.15m in order through R-301 through R-305. After this change, we were able to slightly lower the capital cost, which then increased our NPV. After this final optimization, we were satisfied with the performance of the reactor train and decided to focus on a different part of our process. After additional changes that included flash vaporization temperature and pressure, feed tray of our distillation column, and condenser temperatures in our distillation column, we were able to increase our NPV to $39 million. This is a significant increase from the -$10.4 million we started with in our base case.

Conclusion

I have now shown why process optimization is so important in chemical engineering. By optimizing a process, we are making sure that we are operating at our greatest potential. This will ensure success in the field. By now the reader should have a firm grasp on the aspects of optimization. Understanding the terminology, strategies, decision variable, and other parts of optimization are vital to success. As shown in the ethylbenzene optimization, we were able to increase the NPV by approximately $50 million. This is a dramatic increase from the starting base case. In order to make sure that a facility is operating near its best, I advise everyone to fully take advantage of the process of optimization.

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APPENDIX

Ethylbenzene Case Study

Hunter Lambert
Alec Mattei
ChE 451: Plant Design I

December 8, 2014

Executive Summary

Our goal for this project is to analyze and optimize a given base case of a plant that is designed to produce ethylbenzene at the OM petrochemical facility. The specifications that we had to meet were to produce 80,000 tonne/yr of 99.8 mol% ethylbenzene that will later be consumed by an on-site styrene plant. The composition of our product ethylbenzene stream must have a maximum of two ppm of diethylbenzene. Our objective function was to maximize the net present value of this plant. After designing and analyzing the given base case, we performed an economic analysis to calculate a net present value of -$10.4 million.

We were then presented with two different changes that we could make to our plant. The first change was to use a new type of catalyst, and the second change was to use a lower grade of benzene feed at a cheaper price. After analyzing these two changes, we were presented with four different options that we could proceed with further. These options were to either proceed with the given base case, the first change alone, the second change alone, or with both changes implemented. After analyzing all of the options, we decided to proceed with both of the changes implemented because it gave us the highest net present value of $31.9 million.

After proceeding with both changes, we investigated areas of concern within our plant. We did this by performing a process condition matrix. Areas of concern within the facility were high temperature and pressure within the reactors, non-stoichiometric feed to the reactors, a high log mean temperature differential within the heat exchangers, and a large pressure drop across one of the valves. All justifications can

be read about further within the report. After performing the process condition matrix, we decided to optimize different parts of the ethylbenzene plant. Areas that we looked to optimize were the reactors, flash drum, and the tower. We investigated parameters such as reactor temperature and pressures, number of reactors, flash drum temperature and pressures, feed tray on our column, and our top tray pressure within the column. When we completed the optimization phase, we had a net present value of $39 million.

We feel very confident in the optimizations we have recommended. In order to maximize the net present value, the changes that we implemented should be followed.

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Introduction

Our goal for this project is to analyze and optimize a given base case of a plant that is designed to produce ethylbenzene at the OM petrochemical facility. We will use the net present value (NPV) as the objective function to determine the optimal process design. The plant design should be for a new, grass roots facility. The specifications that we must meet are to produce 80,000 tonne/yr of 99.8 mol% ethylbenzene (EB) that will later be consumed by an on-site styrene plant. The main reaction that forms ethylbenzene is a 1:1 reaction of benzene and ethylene. EB and ethylene can react together to make diethylbenzene (DEB). DEB is an unwanted by-product and will cause complications later in the styrene process. Therefore, we must ensure that the product stream contains less than 2 parts per million. Also, DEB and ethylene react together to form tri- and higher ethylbenzenes. In order to minimize these additional reactions, the catalyst manufacturer has instructed us to keep the benzene to ethylene feed to the reactor train at a molar ratio of 8:1.

We approached the optimization of this process by first analyzing the base case that was given to us. The first step in analyzing the base case was to look at the economic potential of the process. The process concept diagram is shown in Figure A-1 below. From the process concept diagram, we calculated that this process has an economic potential of approximately \$0.39 per kilogram of ethylbenzene produced. Based on our set production rate of 80,000 tonnes per year of our product ethylbenzene stream, the economic potential is approximately \$3,500 per hour. Next, using the simulation software Pro/II, we simulated the process to determine needed raw materials, utilities, and to aid in equipment sizing. From these results, we determined the NPV for the given base case.

We will use this NPV as a comparison to our optimizations to determine if the changes we made are profitable.

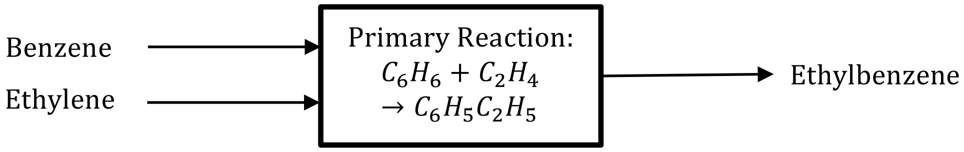


Figure A-1. Process concept Diagram

Initially in the optimization process, we evaluated the two changes that were proposed to us in the description of the case study. These changes included looking at a new type of catalyst and lower grade of benzene feed. After analyzing these two changes, we used a process condition matrix to determine any possible locations for optimization. A few of the optimizations we evaluated were reactor operating conditions, flash drum conditions, and the distillation column conditions. We evaluated our results by simulating the changes made and then comparing the new NPV to our original base case NPV. The process that had the highest NPV is the process that we chose as our optimized case.

Throughout the optimization of the process, we made many assumptions in order to simplify the analysis of our process. We assumed that the land costs were negligible, and the design for the process would be for a new, grass-roots facility. We also assumed that the taxation rates would be 45% per year for the duration of the project. The construction period is two years with a distribution of 60% at the end of year one and 40% at the end of year two. The project would last for twelve years after the construction period ended which would occur at the beginning of year three. The capital investment will depreciate under the MACRS 7 year category. After the twelve years that the project lasts, we assumed that the salvage value is 10% of the fixed capital investment. We also assumed that the labor costs would increase at a rate of 3% per year. In order to calculate the net present value of the plant, we assumed a minimum acceptable rate of return (MARR) of 12%. We assumed that the costs for our raw materials, products, and utilities would stay constant for the duration of the project.

Results and Discussion

Base Case-Process Description

A process flow diagram for the ethylbenzene base case is located in Figure A-2 succeeding the process description. The stream flow table is located in Table A-1 following the process flow diagram. In this process, benzene is fed to a process vessel (V-301) where it is to be mixed with recycled benzene. The feed stream is 97% benzene by composition with the balance toluene. From V-301, the stream is pumped up to 2000 kPa and fed to a fired heater (H-301). Here, the benzene stream is heated up to 400 °C. The benzene stream leaving the fired heater is then mixed with a fraction of the ethylene feed. The feed ethylene stream is 93% ethylene by composition with the balance ethane. The mixed streams then enter a reactor train consisting of three adiabatic packed bed reactors. A list of the four reactions that occur in the reactors are presented below:

$C_6H_6 + C_2H_4 \rightarrow C_6H_5C_2H_5$ (Reaction 1)
Benzene Ethylene Ethylbenzene

$C_2H_4 + C_6H_5C_2H_5 \rightarrow C_6H_4(C_2H_5)_2$ (Reaction 2)
Ethylene Ethylbenzene Diethylbenzene

$C_6H_6 + C_6H_4(C_2H_5)_2 \rightarrow C_6H_5C_2H_5$ (Reaction 3)
Benzene Diethylbenzene Ethylbenzene

C_6H_5CH3 + $2(C_2H_4)$ è $C_6H_5C_2H_5$ + C_3H_6 (Reaction 4)
Toluene Ethylene Ethylbenzene Propylene

The effluent from the first reactor (R-301) mixes with a portion of the ethylene feed. This mixed stream is then sent to a heat exchanger (E-301) to be cooled to 380 °C. After E-301, the stream enters R-302 to be reacted further. Prior to being sent to R-303, the process stream is mixed with the remaining ethylene feed and cooled to 380 °C by E-302. E-301 and E-302 both produce high-pressure steam (HPS) that can later be used for heat integration in the styrene plant. The reactor effluent from R-303 is then sent to three more heat exchangers, E-303, E-304, and E-305. HPS and low-pressure steam (LPS) are generated in E-303 and E-304, respectively. E-303 cools the stream down to 280 °C and E-304 cools the stream down to 170 °C. The final heat exchanger cools the process stream down to 80 °C. After leaving E-305, the cooled process stream is sent through a valve to bring the pressure down to 110 kPa. The large pressure drop across the valve causes a portion of the stream to be vaporized and requires it to be sent to a two-phase separator (V-302). The vapor that comes out of the top can be used as fuel for the fired heater. The liquid stream that comes out of the bottom of V-302 is sent to the first distillation column (T-301). T-301 separates benzene and more volatile chemicals out the top and ethylbenzene and diethylbenzene out the bottom. The overhead stream comprised primarily of benzene is recycled to the beginning of the process to mix with the benzene feed stream at V-301. The bottoms from T-301 are sent to the second distillation column (T-302). T-302 separates ethylbenzene in the overhead and diethylbenzene in the bottoms. Our final ethylbenzene product is produced at 90.592 kmol/hr and a purity of 99.8% by mole ethylbenzene. This translates to 80,000 tonne/yr when a stream factor of 0.95 is applied. The bottoms from T-302 contain the unwanted by-product DEB. The

DEB is mixed with a portion of the recycled benzene from T-301 and sent to H-301. The effluent from H-301 is sent to a fourth adiabatic packed bed reactor (R-304). The benzene and DEB are reacted together to convert the DEB to EB. This reactor effluent is then mixed with the R-303 effluent stream before E-303.

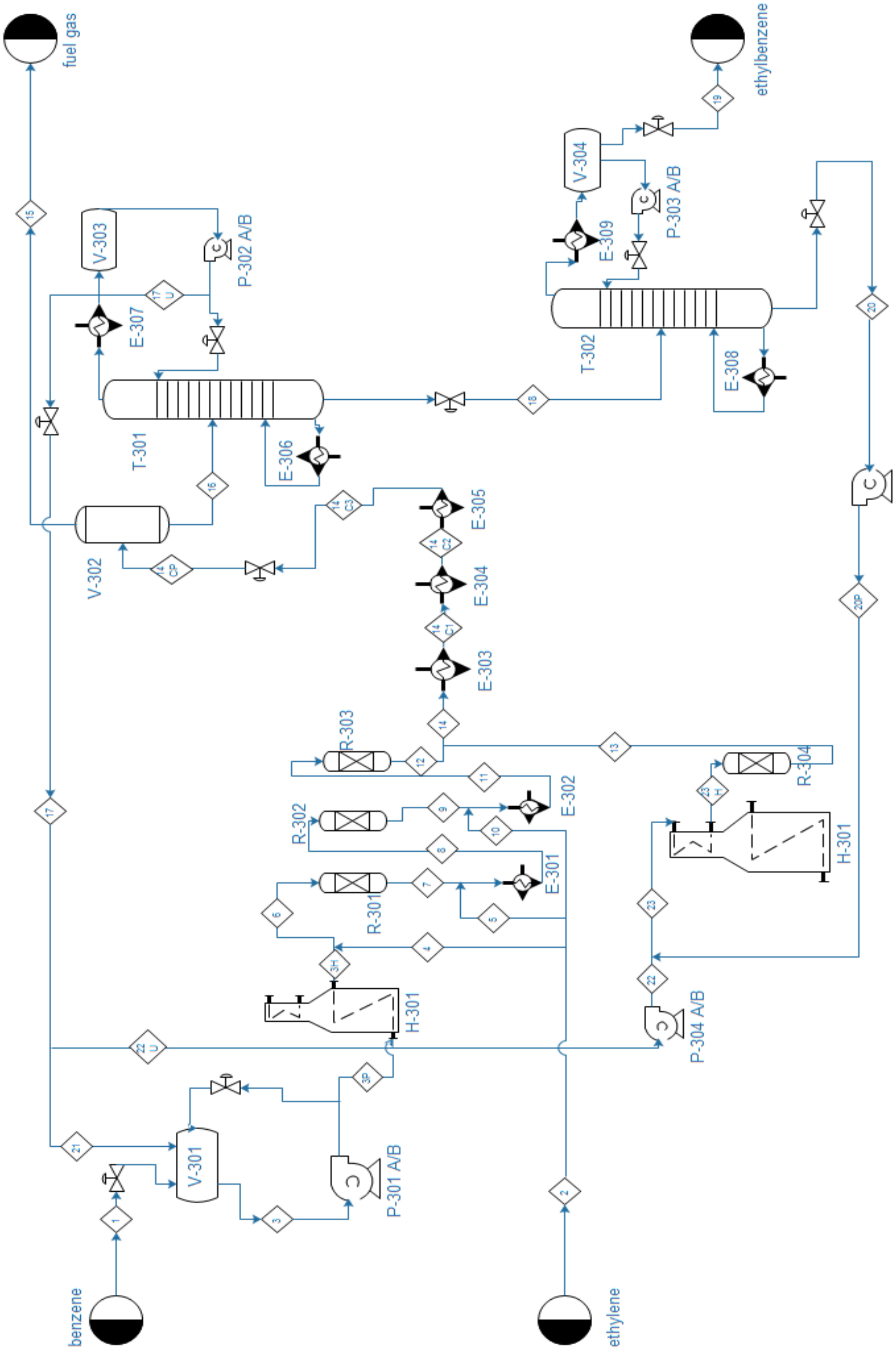


Figure A-2. Base Case Process Flow Diagram

Table A-1. Base Case Stream Flow Table

Stream No.	1	2	3	3P	3PH	4	5
Temperature (°C)	25.0	25.0	39.0	40.8	400.0	25.0	25.0
Pressure (kPA)	110.0	2000.0	105.0	2000.0	2000.0	2000.0	2000.0
Mole Fraction Vap.	0.0	1.0	0.0	0.0	1.0	1.0	1.0
Molar Flow Rate (kmol/hr)	101.0	101.9	233.1	233.1	233.1	30.6	35.7
Mass Flow Rate (kg/hr)	7932.0	2873.8	18180.7	18180.7	18180.7	862.2	1005.8
Flow Rates (kmol/hr)							
ETHYLENE	0.00	94.79	0.06	0.06	0.06	28.44	33.18
ETHANE	0.00	7.13	0.86	0.86	0.86	2.14	2.50
PROPYLENE	0.00	0.00	1.08	1.08	1.08	0.00	0.00
BENZENE	97.97	0.00	227.76	227.76	227.76	0.00	0.00
TOLUENE	3.03	0.00	3.03	3.03	3.03	0.00	0.00
ETHYLBENZENE	0.00	0.00	0.35	0.35	0.35	0.00	0.00
DIETHYLBENZENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Stream No.	6	7	8	9	10	11	12
Temperature (°C)	382.4	440.0	380.0	453.8	25.0	380.0	449.2
Pressure (kPA)	1985.0	1970.0	1960.0	1945.0	2000.0	1935.0	1920.0
Mole Fraction Vap.	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Molar Flow Rate (kmol/hr)	263.7	239.4	275.1	241.6	35.7	277.3	244.0
Mass Flow Rate (kg/hr)	19042.9	19042.9	20048.7	20048.7	1005.8	21054.5	21054.5
Flow Rates (kmol/hr)							
ETHYLENE	28.50	1.20	34.38	0.89	33.18	34.06	0.75
ETHANE	3.00	3.00	5.50	5.50	2.50	8.00	8.00
PROPYLENE	1.08	4.07	4.07	4.11	0.00	4.11	4.11
BENZENE	227.76	206.57	206.57	173.39	0.00	173.39	140.44
TOLUENE	3.03	0.04	0.04	0.00	0.00	0.00	0.00
ETHYLBENZENE	0.35	24.40	24.40	57.40	0.00	57.40	89.98
DIETHYLBENZENE	0.00	0.13	0.13	0.36	0.00	0.36	0.72

Table A-1. Base Case Stream Flow Table (cont'd)

Stream No.	13	14	14C1	14C2	14C3	14C3P	15
Temperature (°C)	500.3	456.0	280.0	170.0	80.0	70.9	70.9
Pressure (kPA)	1988.0	1920.0	1920.0	1920.0	1920.0	110.0	110.0
Mole Fraction Vap.	1.0	1.0	1.0	0.0	0.0	0.1	1.0
Molar Flow Rate (kmol/hr)	42.2	286.2	286.2	286.2	286.2	286.2	21.5
Mass Flow Rate (kg/hr)	3341.9	24396.4	24396.4	24396.4	24396.4	24396.4	1216.9
Flow Rates (kmol/hr)							
ETHYLENE	0.00	0.75	0.75	0.75	0.75	0.75	0.68
ETHANE	0.26	8.26	8.26	8.26	8.26	8.26	7.13
PROPYLENE	0.33	4.45	4.45	4.45	4.45	4.45	3.03
BENZENE	39.13	179.57	179.57	179.57	179.57	179.57	9.78
TOLUENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLBENZENE	2.48	92.46	92.46	92.46	92.46	92.46	0.86
DIETHYLBENZENE	0.00	0.72	0.72	0.72	0.72	0.72	0.00

Stream No.	16	17	17U	18	19	20	20P
Temperature (°C)	70.9	49.5	49.6	142.9	139.3	164.6	166.6
Pressure (kPA)	110.0	105.0	110.0	120.0	110.0	140.0	2000.0
Mole Fraction Vap.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Molar Flow Rate (kmol/hr)	264.7	172.7	172.7	92.2	90.6	1.6	1.6
Mass Flow Rate (kg/hr)	23179.5	13397.0	13397.0	9806.4	9612.8	193.6	193.6
Flow Rates (kmol/hr)							
ETHYLENE	0.08	0.08	0.08	0.00	0.00	0.00	0.00
ETHANE	1.13	1.13	1.13	0.00	0.00	0.00	0.00
PROPYLENE	1.42	1.42	1.42	0.00	0.00	0.00	0.00
BENZENE	169.79	169.66	169.66	0.18	0.18	0.00	0.00
TOLUENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ETHYLBENZENE	91.60	0.46	0.46	91.32	90.41	0.91	0.91
DIETHYLBENZENE	0.72	0.00	0.00	0.72	0.00	0.72	0.72

Table A-1. Base Case Stream Flow Table (cont'd)

Stream No.	21	22	22U	23	23H
Temperature C	49.5	51.0	49.5	58.1	500.0
Pressure (kPA)	105.0	2000.0	105.0	2000.0	2000.0
Mole Fraction Vap.	0.0	0.0	0.0	0.0	1.0
Molar Flow Rate in kg-mol/hr	132.1	40.6	40.6	42.2	42.2
Mass Flow Rate in kg/hr	10248.7	3148.3	3148.3	3341.9	3341.9
Flow Rates (kmol/hr)					
ETHYLENE	0.06	0.02	0.02	0.02	0.02
ETHANE	0.86	0.26	0.26	0.26	0.26
PROPYLENE	1.08	0.33	0.33	0.33	0.33
BENZENE	129.79	39.87	39.87	39.87	39.87
TOLUENE	0.00	0.00	0.00	0.00	0.00
ETHYLBENZENE	0.35	0.11	0.11	1.02	1.02
DIETHYLBENZENE	0.00	0.00	0.00	0.72	0.72

Base Case-Equipment and Utilities

After the base case was simulated in Pro/II and the specifications were met, we calculated the sizes required for all of our equipment. All equations used in calculating the sizes for the equipment can be found in Appendix 5. In order to calculate the most accurate results from Pro/II, we had to choose the most appropriate thermodynamic model. We chose to use SRK Simsci because the SRK model is particularly good for light hydrocarbons at high temperature. We chose to use the Simsci add-on to the SRK model because it is recommended when aromatics are part of the process. All heuristics for our sizing came from chapter 11 in "*Turton*".

Our vessels were sized according to the hold-up time required by the function of each vessel. For example, if a vessel is functioning as a feed drum for another piece of equipment, there should be a hold-up time of approximately ten minutes. A liquid volume of 50% was required for each vessel. One last heuristic used in order to determine the length and diameter of the vessel was to take the ratio of length to diameter to be three. Table A-2 shows the calculated sizing for each vessel.

Table A-2. Vessel Equipment Sizing

Vessel #	Orientation	Length (m)	Diameter (m)
V-301	Horizontal	6.23	2.08
V-302	Vertical	4.75	1.58
V-303	Horizontal	3.59	1.20
V-304	Horizontal	3.58	1.15

Towers were sized using the data acquired in the Pro/II simulation. Shortcut columns were used to find the minimum number of trays for the type of separation we are trying to perform. The actual number of trays required was found using:

$$N_{act} = \frac{2\, N_{min}\, x\ 1.1}{\eta} \qquad (1)$$

Where 1.1 represents a 10% safety factor that is suggested in towers and η is the efficiency which is 75% in this case. In order to calculate the height of our tower, we used the heuristic that each tray should be spaced about 0.55 meters apart and the number of trays. We then used the vapor flow rate through the column to calculate the diameter needed to ensure the tower would not flood or weep. Table A-3 shows the calculated sizes for both T-301 and T-302.

Table A-3. Tower Equipment Sizing

Tower #	# of Trays	Diameter (m)	Height (m)
T-301	23	2.13	15.34
T-302	31	1.43	19.81

Heat exchangers were sized using Pro/II. The first step in order to determine the area of each exchanger was to determine whether or not there was a phase change taking place in the exchanger. If there was no phase change, then only one exchanger for the sensible heat change was needed to find the correct area of heat transfer. If there was a phase change, such as in E-301 when boiler feed water (bfw) is converted to HPS, then two heat exchangers were needed. One heat exchanger is needed for the sensible area of heat transfer and another for the latent area of heat transfer. Therefore, the summation of these two areas gives us total area that the heat exchanger needs to be. For the case of E-304, four heat exchangers were needed to simulate the area needed. This is because not only do we have bfw converting to LPS, but our process stream is also being condensed. This means that we have to calculate two sensible heat areas and two latent areas. Table A-4 shows the calculated duties and areas for each exchanger.

Table A-4. Exchanger Equipment Sizing

H/E #	Type	Duty (GJ/hr)	Area (m^2)
E-301	Floating Head	1.81	53.92
E-302	Floating Head	2.66	75.67
E-303	Floating Head	9.87	382.62
E-304	Fixed Head	12.09	892.29
E-305	Floating Head	4.58	17.99
E-306	Fixed Head	10.10	143.91
E-307	Floating Head	9.27	105.26
E-308	Fixed Head	5.51	48.60
E-309	Floating Head	5.58	17.39

Pump powers and the fired heater duty were found by using the Pro/II simulation and then dividing by the efficiency to find the actual power. Using the heuristics, we were able to find the efficiency for the pumps and fired heater. The reactor length and diameters were given to us in the case study information. Table A-5 shows the equipment information for the fired heater, pumps, and the reactors.

Table A-5. Fired Heater, Pumps, and Reactors Equipment Sizing

Equipment	Duty (GJ/hr)	Power (kW)	Length (m)	Diameter (m)
H-301	30.15	N/A	N/A	N/A
P-301	N/A	24.71	N/A	N/A
P-302	N/A	1.00	N/A	N/A
P-303	N/A	1.00	N/A	N/A
P-304	N/A	0.30	N/A	N/A
P-305	N/A	3.62	N/A	N/A
R-301	N/A	N/A	11.00	1.72
R-302	N/A	N/A	12.00	1.85
R-303	N/A	N/A	12.00	1.97
R-304	N/A	N/A	5.00	0.95

Next, after calculating the equipment sizes, we used Pro/II to calculate the utilities need for the process. All of the energy required and costs for each are shown below in Table A-6.

Table A-6. Utility Information for Base case

Equip. ID	Duty (GJ/hr)	Shaft Power (kW)	Cost ($/yr)
P-301	-	24.71	$ 12,400
P-302	-	1.00	$ 500
P-303	-	1.00	$ 500
P-304	-	1.00	$ 500
P-305	-	3.62	$ 1,800
E-301	1.81	-	$ (266,300)
E-302	2.66	-	$ (391,700)
E-303	9.87	-	$ (1,454,300)
E-304	12.09	-	$ (1,413,700)
E-305	4.58	-	$ 13,500
E-306	10.10	-	$ 1,181,500
E-307	9.27	-	$ 27,300
E-308	5.51	-	$ 811,700
E-309	5.58	-	$ 16,400
H-301	30.15	-	$ 2,784,900
		Total =	$ 1,325,000

Base Case-Pricing

After determining the sizing of the equipment and needed utilities, we began performing an economic analysis of the base case. First, there are 16 pieces of equipment that will need some type of supervision by operators. We were able to show that we will need 15 operators to run this facility using:

$$\frac{Operators}{Shift} = (6.29 + 0.23\ Pieces\ of\ Equipment)^{0.5} \qquad (2)$$

$$Total\ Operators = \frac{Operators}{shift}\, x\ 4.5 \qquad (3)$$

Using "Capcost", an equipment pricing software, and the equipment sizing calculations, we were able to calculate the total bare module cost to be approximately $5.96 million. Next, we calculated the annual revenue and costs.

Table A-7. Pricing for Base Case per year

Total Revenue	$112,700,000
Raw Materials	$85,800,000
Cost of Utilities	$1,300,000
Cost of Operating Labor	$900,000

After doing a cash flow statement, our NPV for the base case process was approximately -$10.4 million. It would take almost 14 years to break even on this project. However, since this is a 12 year project, we would never be able to break even. After investigating the base case, we then looked into further ways to improve this process to increase the NPV.

Proposed Changes

In the case study description, two changes were proposed that we evaluated. Change one was to try out a new catalyst that would suppress the ethylation of EB to DEB. The second change that was proposed was to purchase a lower grade of benzene for a reduced price.

First, we analyzed how the new catalyst would change our process. This new catalyst has a cost of \$8/kg and an expected lifetime of four years. It has a maximum operating temperature of 500°C, pack void fraction of 0.4, and a bulk density of 1250 kg/m^3. Exploring this option in Pro/II, we were able to see that by using this new catalyst, we were able to significantly lower the quantity of DEB in the effluent from the reactor train. The NPV for this change increased to approximately -\$9.3 million. Therefore, using the new proposed catalyst is more economical than the base case.

Change two gave us the opportunity to purchase a lower grade of benzene that contains 10% toluene for \$0.85/kg. After updating the information in Pro/II, it was easy to see that this would be a very profitable change. There was an NPV increase to approximately \$27.1 million. There were no significant changes that needed to be made to the process. The equipment sizes and duties of equipment changed slightly, but they were very insignificant compared to our base case.

Now that both change one and two had been evaluated and both increased the NPV compared to the base case, we were faced with four different options we could make. We could make change one, change two, neither, or both. In order to decide on what option we would choose, we wanted to look at the combination of the two changes to see how our NPV changed. When both of the changes were implemented, our NPV increased to approximately $31.9 million. Implementing both changes increased our NPV the largest and therefore we progressed the optimization with both changes being used.

Optimization

After looking at the base case, we realized that this project needed much improvement. The NPV was negative, and we would never be able to break even on the project. Change 2 increased the NPV up to around $27.1 million. This significant increase is due to the fact that the raw materials are one of the main factors when it comes to the total costs of the plant. This can be seen by looking at the sensitivity analysis for the base case in Appendix 3. This means that it does not take much difference in raw materials for the NPV to be drastically impacted. Even though we increase the amount of feed that is needed to produce 80,000 tonne/yr of EB, the cheaper price that we are able to buy the feed justifies the change. After deciding to do both changes, we were able to increase our NPV to approximately $31.9 million. We knew that there were still things in the facility that could be optimized. To narrow our focus on certain parts of the process to optimize, we decided to do a process condition matrix. Our process condition matrix can be found Appendix 4.

From the process condition matrix, the temperature, pressure, and non-stoichiometric feed was of concern in our reactors. If the reactor temperature rises above 400 °C, special material must be used in the construction of the reactor. In order to determine if we could lower our reactor temperatures, we decided to run a case study on the entire reactor train in Pro/II. This case study would compare the selectivity of EB to DEB and the conversion of benzene from a temperature range of 200°C to 435°C. We went up to 435°C because it brought the effluent from each reactor to just below 500°C.

We did not want to pass 500°C because our catalyst manufacturer has made it clear this is the maximum operating temperature of the catalyst without catalyst poisoning taking effect. The result of this case study can be seen in Figure A-3.

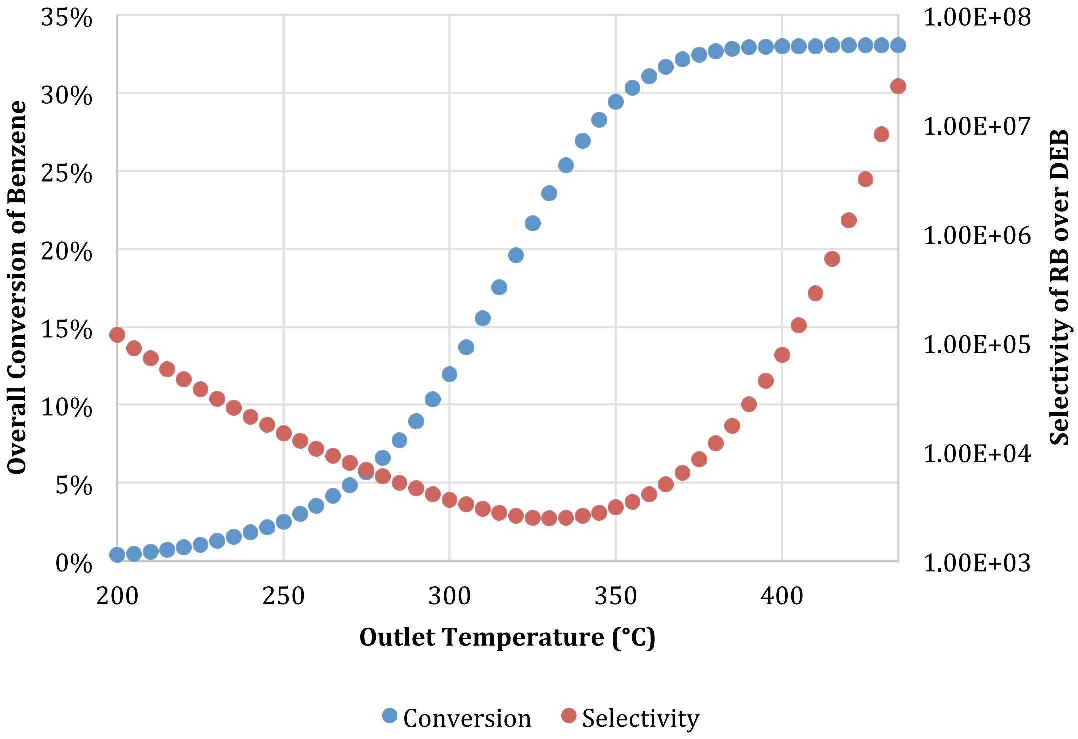


Figure A-3. Conversion & Selectivity vs. Temperature of Reactor Train

It can be seen in Figure A-3, that as we increase the temperature, both the conversion and selectivity increase. If we try to eliminate the use of special materials, we would need stay below 400°C at all points in the reactor. In order to do this, our feed would need to be approximately 340°C to each reactor. From Figure 3, we see that in this range the selectivity is about four orders of magnitude less than what it would be at maximum temperatures and the conversion is about 6% less. To determine if lowering the temperature is more economical, we calculated the length of each reactor to produce the required amount of EB at the lower temperature. Our reactor lengths would have to be approximately three times as long. We compared the cost of the larger reactors to the special material reactors to determine which was more profitable. We determined that stainless steel should be used as the special material for the reactors at higher temperatures from "*Perry's Chemical Engineering Handbook*". After comparing the two, we decided to operate our reactor train at a temperature that maximizes the effluent stream out of each reactor to just below 500 °C to give maximum conversion and selectivity. This was cheaper than trying to lower the operating temperature and making the reactors larger.

Next, we decided to investigate the affect that pressure had on the reactor train. Heuristics tell us that if we do not operate under 10 bar that we will have to build thicker walled equipment. We ran a case study comparing the selectivity of EB to DEB and the conversion of benzene from 1000 kPa to 2000 kPa. The chart from this case study is presented in Figure A-4.

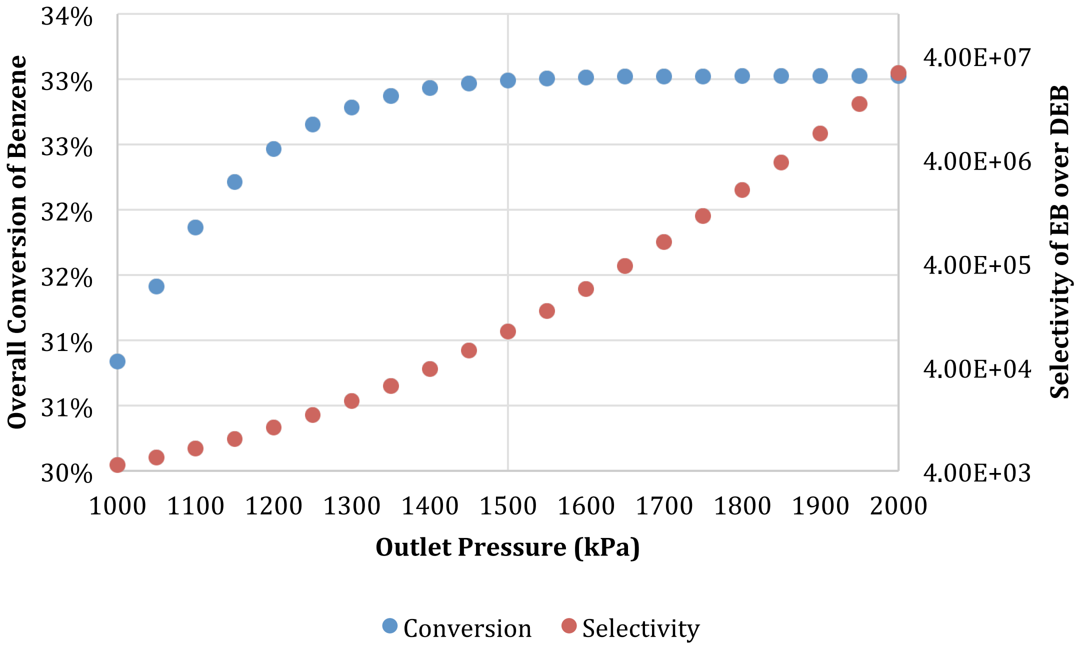


Figure A-4. Overall Conversion and Selectivity vs. Pressure

The conversion does not vary much with this decrease in pressure. However, there is a significant decrease in the selectivity of EB when we decrease pressure. We would have to increase the reactor lengths by nearly three times their original length to meet our specification of 80,000 tonne/year of EB. Based on the cost for the thicker walled reactors and the cost of the larger reactors, it was more economical to run the reactors at high pressure.

Another heuristic for the reactors is to have a stoichiometric feed. This could be done, however, we would create more harmful by-products in our facility. The catalyst manufacturer told us to keep an 8:1 benzene to ethylene mole ratio to ensure no tri- or higher ethylbenzenes were produced in our process. Because we do not have the reaction kinetics for these types of reactions, we decided to keep the 8:1 ratio into the reactor train.

After deciding to run maximum temperature and high pressure in the reactors, we noticed the effluent stream contained practically no DEB. The temperature and pressure conditions along with the new catalyst allowed us to take an opportunity to optimize the process by removing the second distillation column and in turn the entire bottom recycle of DEB. Removing this part of the process led to a smaller fired heater and eliminated the fourth adiabatic plug flow reactor. Also, T-302 was eliminated, which in turn eliminated E-308 and E-309 from the process. The NPV of the process increased to approximately \$32.4 million and we decide to progress our optimizations with this change due to the increased NPV.

Now that we have our reactor temperatures and pressures defined, we wanted to explore the option of putting in a fourth reactor in the reactor train. Theoretically, we believed that adding in another reactor to the reactor train would in turn increase our conversion of benzene to EB and the selectivity of EB. With only three reactors in the reactor train, we had a selectivity of EB to DEB of 3.5×10^7 and a conversion of benzene of 33%. When we put in a fourth reactor, our selectivity decreased to 7.2×10^5 but our conversion increased to 40%. Even though our selectivity decreased, practically no DEB was still produced. Due to the conversion increasing by about 7 %, we were able to decrease the amount of raw materials that was needed for our process because we were losing less benzene in the fuel gas. However, we had to add in another heat exchanger so that effluent from R-303 was lowered to the appropriate temperature for the newly added reactor. This extra heat exchanger will cost us in capital expenses, however it will make HPS, which decreases the utility cost. This overall process increased the NPV to approximately $36.8 million even though our equipment cost slightly increased. Again this corresponds to the sensitivity analysis which shows that raw material costs strongly effects the NPV, where utility costs does not show much of an effect.

Our final reactor variable that we decided to investigate was the reactor lengths for each reactor. We believed that there would be an optimum length at the operating temperature and pressure that would reduce our raw materials enough to increase the NPV. An exploration of conversion of benzene versus the length of the each reactor allowed us to determine the appropriate length for each reactor. The case studies for all reactors in the train are shown below in Figures A-5 through A-8.

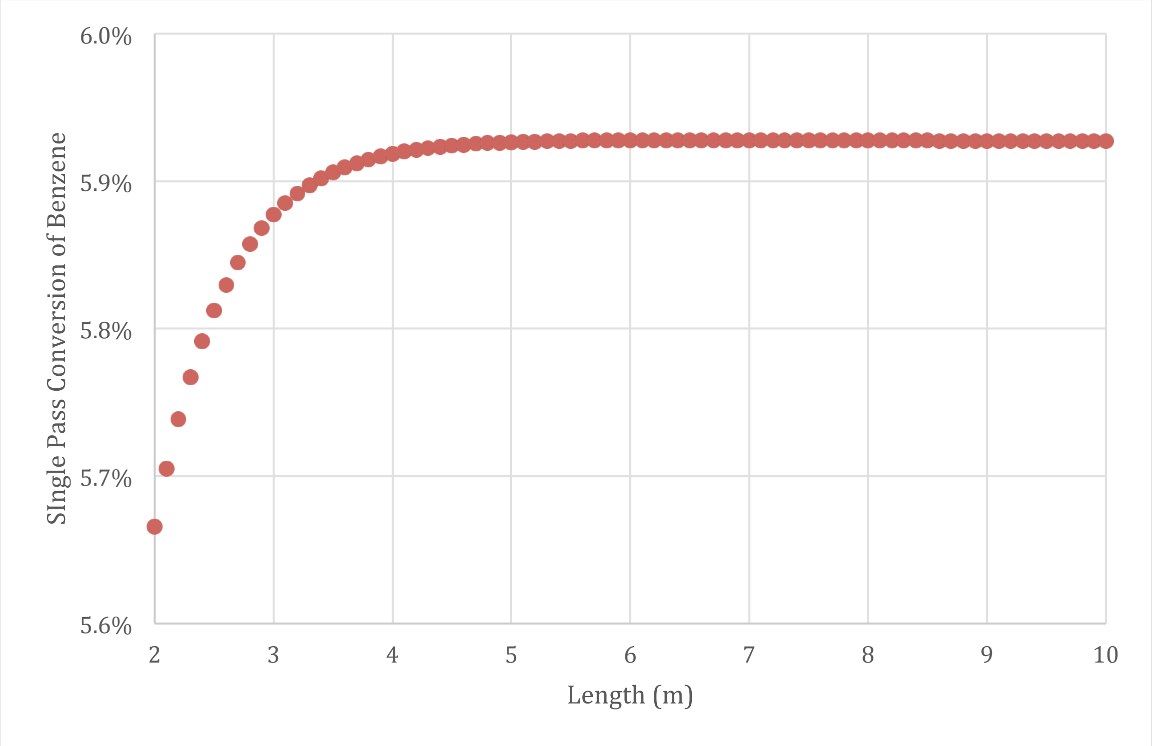


Figure A-5. R-301 Conversion as a Function of Length

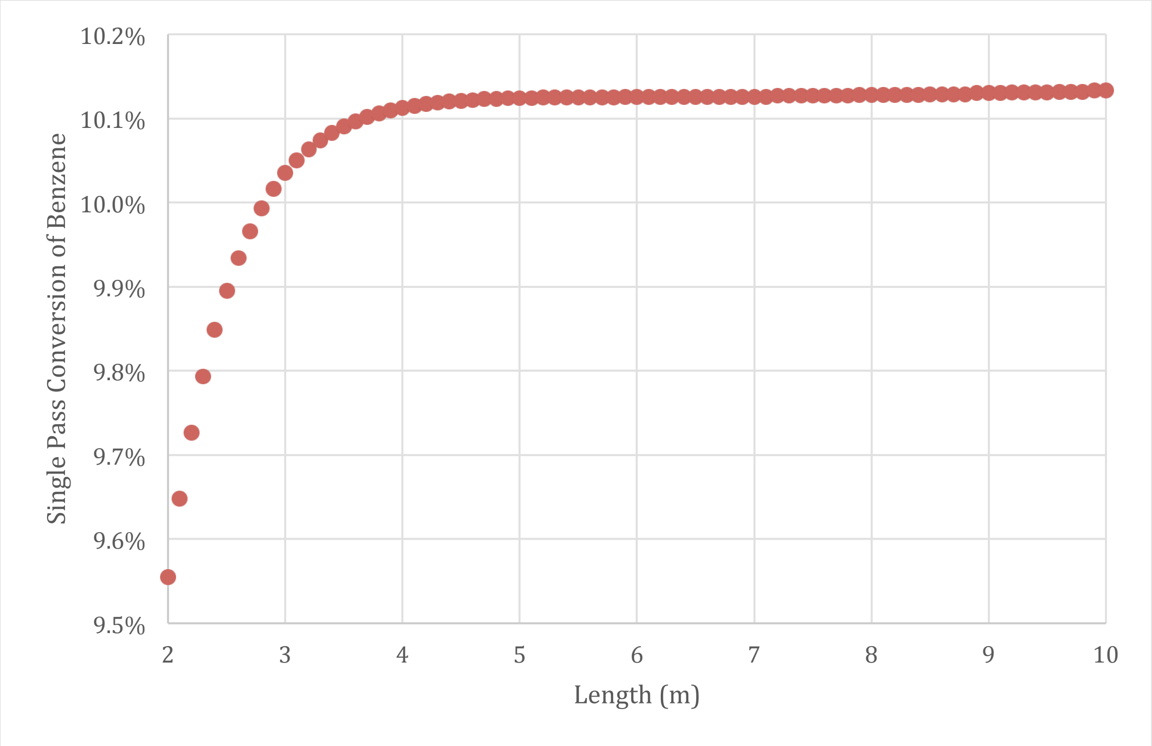


Figure A-6. R-302 Conversion as a Function of Length

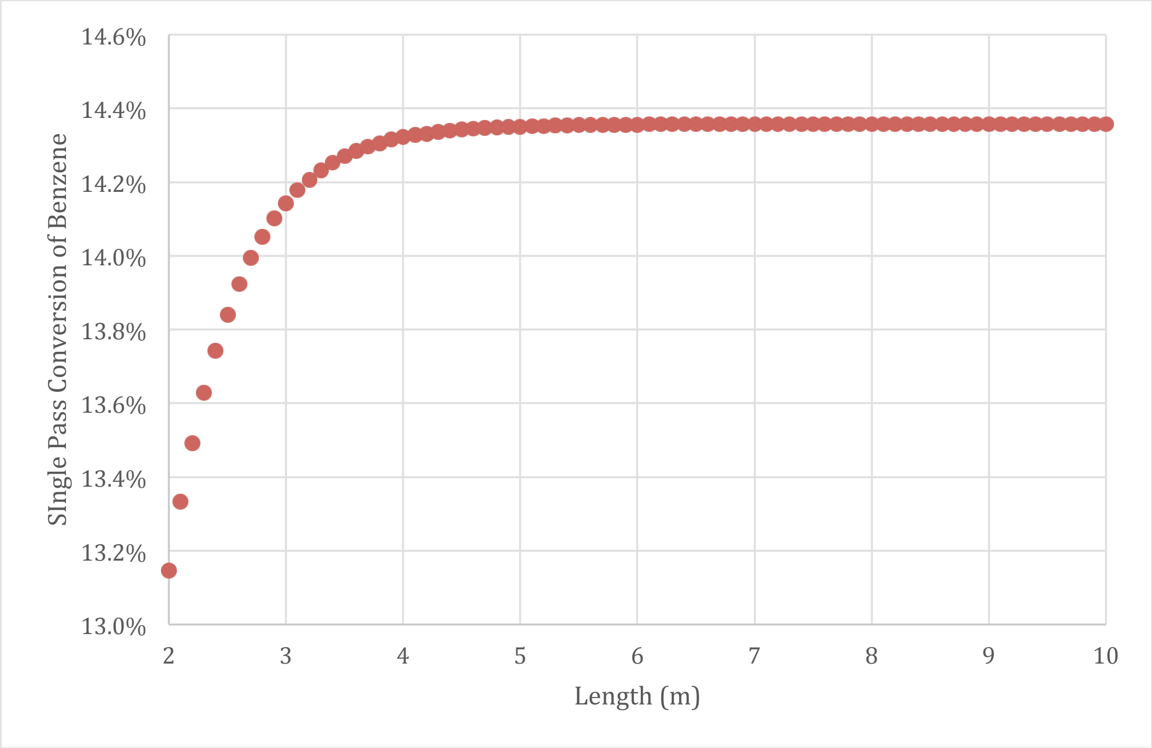


Figure A-7. R-303 Conversion as a Function of Length

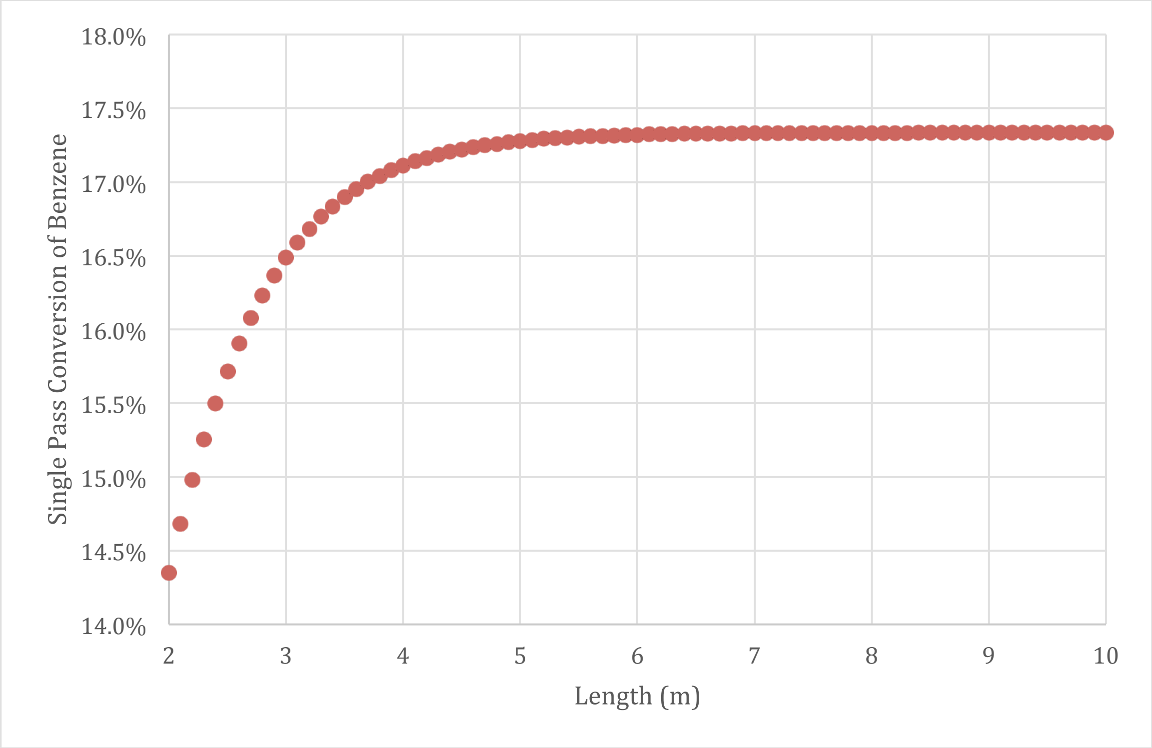


Figure A-8. R-305 Conversion as a Function of Length

After looking at the figures, we determined there was a range for reactor length where conversion would stay constant. In order to minimize the capital costs for our reactors and catalyst cost, we determined that our optimum lengths in Pro/II would be 4.95m, 5.36m, 5.84m, and 6.15m in order through R-301 through R-305. After this change, we were able to slightly lower the capital cost, which then increased our NPV. After this final optimization, we were satisfied with the performance of the reactor train and decided to focus on a different part of our process.

In the initial process condition matrix, we found a few instances where our log mean temperature difference (ΔT_{LM}) was greater than 100 °C. If this is the case, we are wasting valuable energy. The heat exchangers that this condition is not met are E-301, E-302, E-303, and E-308. The solution to this problem was to integrate heat better within the facility. However, as per the scope of this case study, we are not to perform heat integration within this process because there will be heat integration with the connected styrene facility. This justifies the reason why our ΔT_{LM} was greater than 100 °C in E-301 through E-303. This still left us with E-308 though. However, this was the reboiler for T-302, which has been removed due to prior optimization steps and is of no concern now.

The final process condition matrix condition that we needed to check was the large pressure drop across the valve directly before the flash vaporizer. Technically, this pressure drop is justified because a liquid is being throttled. However, we wanted to look at opportunities to decrease the pressure at a point where the process stream is still a vapor and therefore capture this work as an electric credit. We moved the turbine from the current valve location to before the series of exchangers where the process stream is a vapor. After the series of heat exchangers, the process stream becomes a liquid, which is unsuitable for a turbine. We updated the process in Pro/II, and found that the NPV decreased because more benzene was flashed off causing a waste of raw materials. After analyzing the results, we also found that the turbine increased our utilities cost by approximately $1.3 million per year. After investigation, we decided to stick with the large pressure drop across the valve. Although we are losing some energy here, it is more economical than trying to put a turbine earlier in the process.

The next step in optimizing our facility was to take a look at our flash drum. We looked at the data and saw that we were losing about 10% of our benzene feed. We decided that if we could change the pressure or inlet temperature, we might be able to lower the loss of benzene. However, we wanted to see how this affected our utilities cost so we decided to look at this over a pressure and temperature range. Using Pro/II, we ran two separate case studies. In each case, we plotted the percent loss of benzene and an objective function that give us a rough estimate for the profit. This objective function includes the revenue from our product stream and fuel gas, the cost for the raw materials, and all utilities. These two case studies are shown in Figures A-9 and A-10.

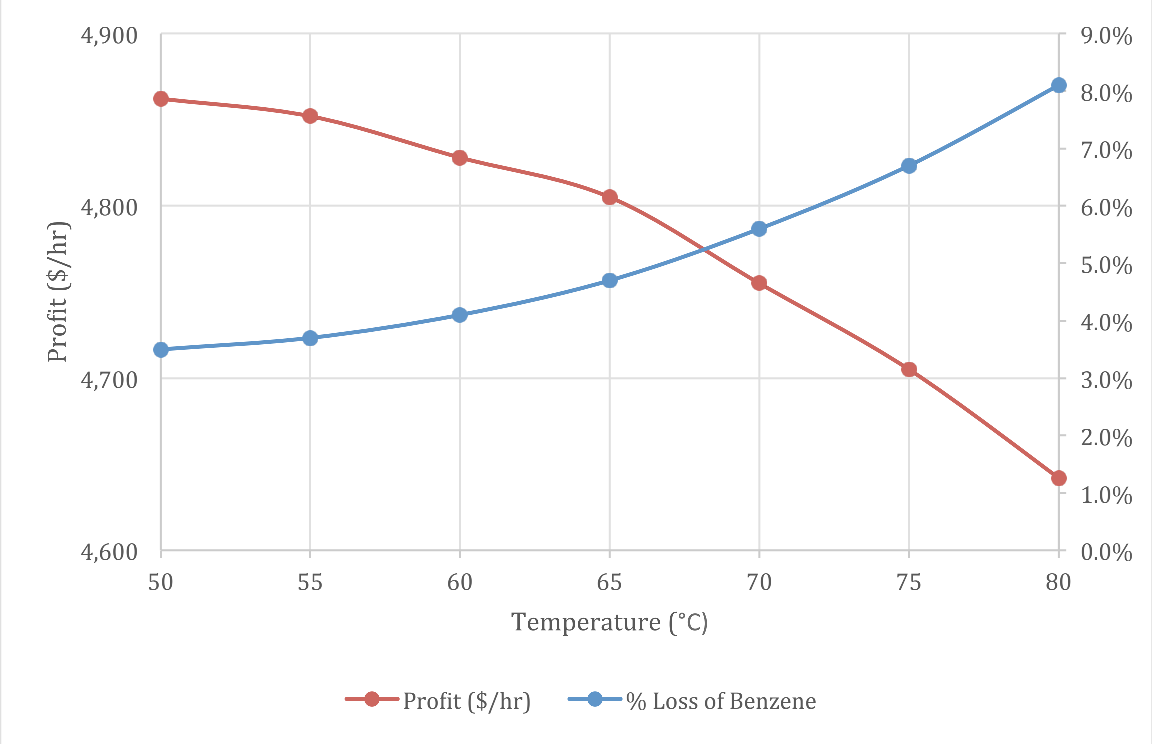


Figure A-9. Temperature Effect on Profit and % Loss of Benzene

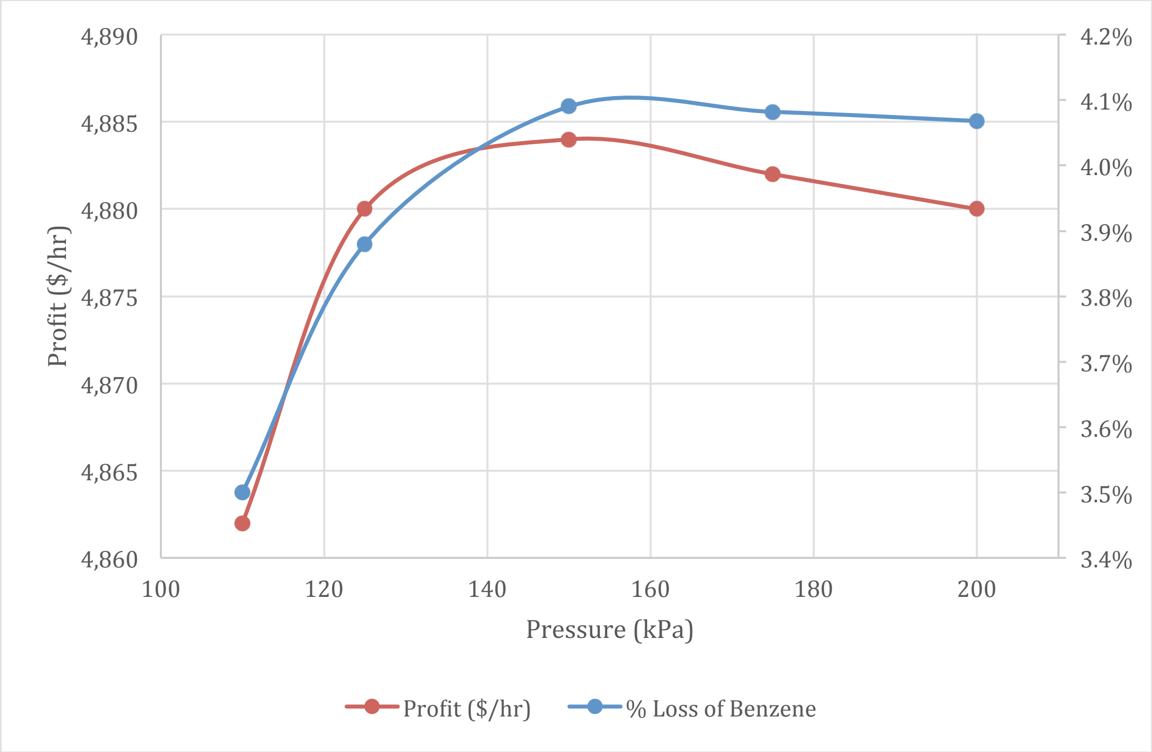


Figure A-10. Pressure Effect on Profit and % Loss of Benzene

In Figure A-9, the percent loss of benzene changes significantly which allows us to see the increase in profit. We used a low temperature of 50 °C so we could maintain a ten degree approach temperature in E-305. Based on the results, we will operate E-305 with an outlet temperature of 50 °C to maximize profit and minimize the loss of benzene. Next, we analyzed Figure A-10 to determine the pressure to operate the flash drum. We found that at approximately 150 kPa, we maximized the profit of the process. This case study was done at the new outlet temperature of E-305. Therefore, we chose to operate the flash drum at a pressure of 150 kPa.

The final piece of equipment that we wanted to explore further was our distillation tower. We were able to determine the number of stages from our shortcut column. However, there were a few variables that we could alter to try and improve the process. One thing that we noticed when we initially ran our simulation is that our process stream coming out of the condenser was at about 14°C. In order to condense this stream, we would have to use some type of refrigeration utility. Using a refrigeration utility would be much more expensive than cooling water. We decided to change the condenser from a total condenser to a partial condenser and see if it would alleviate our problem. After making this change we found that our process stream out of the condenser is approximately 49 °C. At this temperature, the 10 °C ΔT_{LM} can be satisfied for cooling water.

The next step in optimizing our tower was to focus on the location of the feed tray. In order to find the most optimal location to minimize costs for our reboiler and condenser, we performed a case study in Pro/II. We set the utility cost of the reboiler and condenser as the objective function and the goal was to minimize this as much as possible. In Figure A-11, we see that the optimal feed tray is tray nine to reduce the utility costs associated with this tower.

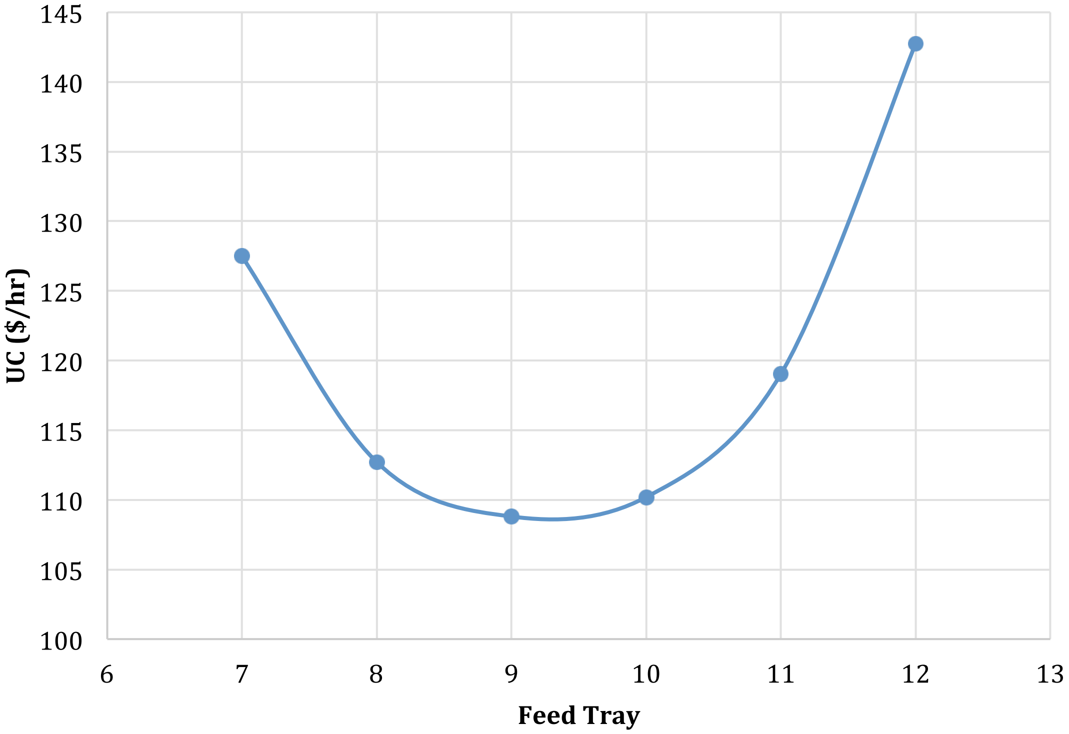


Figure A-11. T-301 Utility Costs as a function of Feed Tray

The last step we looked at in optimizing our tower was the top tray pressure. For this variable, we used the optimizer function in Pro/II with the objective function as the reboiler and condenser utility cost. However, after multiple iterations, there was no change in the optimal pressure, which lead us to the conclusion that we should maintain the top tray pressure of 110 kPa.

Final Optimized Process Description

A PFD and stream flow table for the optimized case are located in Figure A-12 and Table A-8, respectively, following the process description. A benzene feed stream is sent to a process vessel (V-301) where it is to be mixed with recycled benzene. The feed stream is 90% benzene by composition and the balance is toluene. From V-301, the stream is pumped up to 2000 kPa and fed to a fired heater (H-301). Here, the feed benzene stream is heated up to 464 °C. The benzene stream leaving the fired heater is then mixed with an ethylene feed. The feed ethylene stream is 93% ethylene by composition and the balance is ethane. The mixed streams then enter a reactor train consisting of four adiabatic packed bed reactors. The effluent from the first reactor (R-301) leaves to be mixed with more ethylene feed. This mixed stream is then sent to a heat exchanger (E-301) to be cooled to 445 °C. After E-301, the stream enters R-302 to react further. Prior to being sent to R-303, the process stream is mixed with a fraction of ethylene feed and cooled to 445 °C by E-302. Prior to being sent to R-305, the effluent from R-303 is mixed with the remaining fraction of ethylene feed, and cooled to 445 °C by E-310. E-301, E-302, and E-310 all produce high-pressure steam (HPS) that can later be used for heat integration in the styrene plant. The reactor effluent from R-305 is then sent to two more heat exchangers, E-303 and E-304. HPS and LPS are generated, respectively. E-303 cools the stream down to 280 °C and E-304 cools the stream down to 170 °C. The process stream is sent to one more heat exchanger (E-305) that cools the process stream down to 50 °C. The cooled process stream is sent through a valve to reduce the pressure to 150 kPa. The pressure drop causes a portion of the stream to vaporize. It is next sent to a two-phase separator (V-302). The vapor that comes out of the top is fuel has that can be sold for a credit and used in the fired heater. The liquid that comes out of the bottom is then sent to the distillation tower (T-301). T-301 separates benzene and more volatile components in the overhead and EB in the bottom. The overhead vapor is sent through a partial condenser (E-307) to cool the overhead to approximately 50 °C. The liquid effluent is mainly composed of benzene, and this stream is sent to be recycled to the beginning of the process to be mixed with benzene feed in V-301. The vapor effluent out of the condenser is mixed with the vapor stream out of the flash that is to be sold as fuel gas. Our ethylbenzene product is produced out of the bottom of T-301 at 90.592 kmol/hr. This translates to 80,000 tonne/yr when a stream factor of 0.95 is applied. This stream has to be cooled down to 139 °C and depressurized to 110 kPA by E-311 before it is sent to the styrene plant.

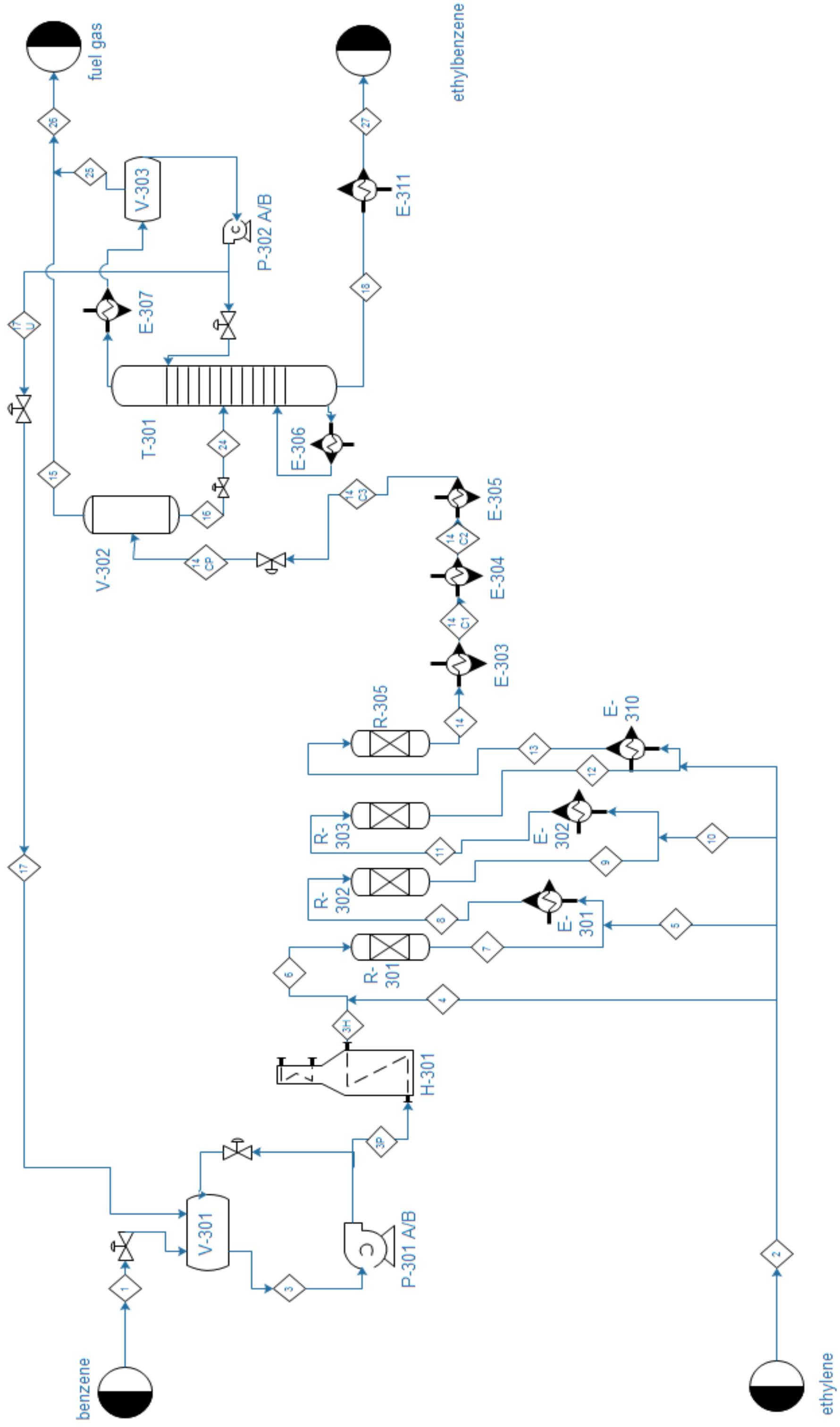


Figure A-12. Optimized Process Flow Diagram

Table A-8. Optimized Case Stream Flow Table

Stream No.	1	2	3	3P	3H	4
Temperature (°C)	25.0	25.0	38.8	40.6	464.0	25.0
Pressure (kPA)	110.0	2000.0	105.0	2000.0	2000.0	2000.0
Mole Fraction Vapor	0.0	1.0	0.0	0.0	1.0	1.0
Total Molar Rate (kmol/hr)	95.3	107.6	213.2	213.2	213.2	26.9
Total Mass Rate (kg/hr)	7577.9	3033.2	16674.9	16674.9	16674.9	758.3
Flow Rates (kmol/hr)						
ETHYLENE	0.00	100.05	0.00	0.00	0.00	25.01
ETHANE	0.00	7.53	0.34	0.34	0.34	1.88
PROPYLEN	0.00	0.00	2.74	2.74	2.74	0.00
BENZENE	85.77	0.00	200.50	200.50	200.50	0.00
TOLUENE	9.53	0.00	9.53	9.53	9.53	0.00
EBENZENE	0.00	0.00	0.09	0.09	0.09	0.00
14EBENZN	0.00	0.00	0.00	0.00	0.00	0.00

Stream No.	5	6	7	8	9	10
Temperature (°C)	25.0	444.7	490.6	444.7	496.2	25.0
Pressure (kPA)	2000.0	1985.0	1970.0	1960.0	1945.0	2000.0
Mole Fraction Vapor	1.0	1.0	1.0	1.0	1.0	1.0
Total Molar Rate (kmol/hr)	26.6	240.1	221.6	248.2	226.2	27.0
Total Mass Rate (kg/hr)	750.7	17433.2	17433.2	18183.9	18183.9	762.1
Flow Rates (kmol/hr)						
ETHYLENE	24.76	25.01	0.00	24.77	0.00	25.14
ETHANE	1.86	2.23	2.23	4.09	4.09	1.89
PROPYLEN	0.00	2.74	9.20	9.20	11.94	0.00
BENZENE	0.00	200.50	188.42	188.42	169.13	0.00
TOLUENE	0.00	9.53	3.06	3.06	0.33	0.00

EBENZENE	0.00	0.09	18.63	18.63	40.66	0.00
14EBENZN	0.00	0.00	0.00	0.00	0.00	0.00

Table A-8. Optimized Case Stream Flow Table (Cont'd)

Stream No.	11	12	13	14	14C1	14C2
Temperature (°C)	444.7	499.7	444.7	497.7	280.0	170.0
Pressure (kPA)	1935.0	1920.0	1910.0	1895.0	1885.0	1875.0
Mole Fraction Vapor	1.0	1.0	1.0	1.0	1.0	0.0
Total Molar Rate (kmol/hr)	253.2	228.4	255.4	230.3	230.3	230.3
Total Mass Rate (kg/hr)	18946.0	18946.0	19708.1	19708.1	19708.1	19708.1
Flow Rates (kmol/hr)						
ETHYLENE	25.14	0.00	25.14	0.01	0.01	0.01
ETHANE	5.98	5.98	7.87	7.87	7.87	7.87
PROPYLEN	11.94	12.26	12.26	12.27	12.27	12.27
BENZENE	169.13	144.63	144.63	119.52	119.52	119.52
TOLUENE	0.33	0.01	0.01	0.00	0.00	0.00
EBENZENE	40.66	65.48	65.48	90.60	90.60	90.60
14EBENZN	0.00	0.00	0.00	0.00	0.00	0.00

Stream No.	14C3	14CP	15	16	17	17U
Temperature (°C)	50.0	43.8	45.6	45.6	50.0	49.7
Pressure (kPA)	1865.0	110.0	150.0	150.0	110.0	105.0
Mole Fraction Vapor	0.0	0.1	1.0	0.0	0.0	0.0
Total Molar Rate (kmol/hr)	230.3	230.3	12.0	218.2	117.9	117.9
Total Mass Rate (kg/hr)	19708.1	19708.1	501.3	19206.8	9097.0	9097.0
Flow Rates (kmol/hr)						
ETHYLENE	0.01	0.01	0.00	0.00	0.00	0.00
ETHANE	7.87	7.87	5.47	2.40	0.34	0.34

PROPYLEN	12.27	12.27	4.99	7.28	2.74	2.74
BENZENE	119.52	119.52	1.43	118.08	114.73	114.73
TOLUENE	0.00	0.00	0.00	0.00	0.00	0.00
EBENZENE	90.60	90.60	0.14	90.46	0.09	0.09
14EBENZN	0.00	0.00	0.00	0.00	0.00	0.00

Table A-8. Optimized Case Stream Flow Table (Cont'd)

Stream No.	18	24	25	26	27
Temperature (°C)	142.7	44.6	50.0	47.4	139.0
Pressure (kPA)	120.0	115.0	110.0	110.0	110.0
Mole Fraction Vapor	0.0	0.0	1.0	1.0	0.0
Total Molar Rate (kmol/hr)	90.6	218.3	9.8	21.9	90.6
Total Mass Rate (kg/hr)	9612.8	19214.9	505.1	1006.4	9612.8
Flow Rates (kmol/hr)					
ETHYLENE	0.00	0.00	0.00	0.01	0.00
ETHANE	0.00	2.40	2.06	7.53	0.00
PROPYLEN	0.00	7.28	4.54	9.53	0.00
BENZENE	0.18	118.13	3.23	4.66	0.18
TOLUENE	0.00	0.00	0.00	0.00	0.00
EBENZENE	90.41	90.50	0.00	0.14	90.41
14EBENZN	0.00	0.00	0.00	0.00	0.00

Optimized Equipment and Utilities

After performing the optimization steps, we felt very confident in the decisions we made. The next step was to simulate the optimized process and recalculate all of our equipment sizes along with the utilities needed. Using Pro/II, we were able to calculate the duty for the heat exchangers and the fired heater along with the power required for the pumps. These values and the costs associated are broken down in Table A-9.

Table A-9. Utilities Needed for the Optimized Case

Equip. ID	Duty (MJ/hr)	Shaft Power (kW)	Cost ($/yr)
P-301	-	22.8	$ 11,400
P-302	-	1.0	$ 500
E-301	1.19	-	$ (174,500)
E-302	1.54	-	$ (226,500)
E-303	10.18	-	$(1,499,200)
E-304	9.81	-	$(1,147,500)
E-305	4.89	-	$ 14,400
E-306	8.75	-	$ 1,023,200
E-307	6.67	-	$ 19,600
E-310	1.83	-	$ (269,600)
E-311	0.08	-	$ 200
H-301	26.10	-	$ 2,171,700
		Total =	$ (76,300)

In the optimized case, we are making money due to the decreased duty in H-301, the removal of E-308 and E-309, and the addition of E-310. After calculating the utilities needed, we determined the equipment sizes for the optimized process.

Using the same calculations as discussed in the base case equipment sizing along with the calculations presented in Appendix A-5, we were able to determine sizes for all of our equipment.

Table A-10. Optimized Case Pump Sizing

Pump #	Material	Type	Power (kW)	Discharge Pressure (kPaG)	# of Spares
P-301	Carbon Steel	Positive Displacement	22.818	1898.675	1
P-302	Carbon Steel	Centrifugal	1.000	8.675	1

Table A-11. Optimized Case Vessel and Reactor Sizing

Vessel #	Orientation	Material	Demister Material	Length (m)	Diameter (m)	Max Pressure (kPaG)
V-301	Horizontal	Carbon Steel	N/A	6.02	2.01	148.68
V-302	Vertical	Carbon Steel	S.S.	4.40	1.47	148.68
V-303	Horizontal	Carbon Steel	N/A	3.15	1.05	198.68
R-301	Vertical	Stainless Steel	N/A	7.35	1.65	2098.68
R-302	Vertical	Stainless Steel	N/A	7.76	1.79	2098.68
R-303	Vertical	Stainless Steel	N/A	8.24	1.95	2098.68
R-305	Vertical	Stainless Steel	N/A	8.55	2.05	2098.68

Table A-12. Optimized Case Tower Sizing

Tower #	Material	Tray Type	Tray Material	# of Trays	Diameter (m)	Height (m)	Max Pressure (kPaG)
T-301	Carbon Steel	Sieve	Carbon Steel	21	2.06	14.23	198.68

Table A-13. Optimized Case Heat Exchanger and Fired Heater Sizing

Heat Exchanger #	Material	Type	Max Pressure (kPaG)	Duty (GJ/hr)	Area (m^2)
E-301	Carbon Steel	Floating Head	2098.68	1.19	25.98
E-302	Carbon Steel	Floating Head	2098.68	1.54	33.28
E-303	Carbon Steel	Floating Head	2098.68	10.18	349.50
E-304	Carbon Steel	Fixed Head	2098.68	9.81	734.75
E-305	Carbon Steel	Floating Head	2098.68	4.89	29.32
E-306	Carbon Steel	Fixed Head	98.68	8.75	123.27
E-307	Carbon Steel	Floating Head	98.68	6.67	77.45
E-310	Carbon Steel	Floating Head	2098.68	1.83	39.25
E-311	Carbon Steel	Floating Head	98.68	0.08	10.15
H-301	Carbon Steel	Non-Reactive	2098.68	26.10	---

After determining the sizes required for all of our equipment, we can begin to calculate the net present value of our optimized case.

Final Optimized Price

Using the equipment sizing described above and Capcost, we determined the total bare module cost for the equipment. The bare module cost for all of the equipment in the optimized case is presented in Table A-14.

Table A-14. Bare Module Cost for the Optimized Process

Equipment ID	Purchased Equipment Cost	Bare Module Cost
E-301	$ 26,600.00	$ 95,200.00
E-302	$ 27,200.00	$ 97,300.00
E-303	$ 77,300.00	$ 277,000.00
E-304	$ 90,900.00	$ 303,000.00
E-305	$ 26,800.00	$ 91,800.00
E-306	$ 36,800.00	$ 121,000.00
E-307	$ 33,200.00	$ 109,000.00
E-310	$ 27,800.00	$ 99,600.00
E-311	$ 28,700.00	$ 94,300.00
H-301	$ 1,070,000.00	$ 2,270,000.00
P-301	$ 24,400.00	$ 99,700.00
P-302	$ 7,090.00	$ 28,200.00
T-301	$ 117,000.00	$ 281,000.00
V-301	$ 22,300.00	$ 67,000.00
V-302	$ 16,800.00	$ 58,200.00
V-303	$ 7,910.00	$ 23,800.00
R-301	$ 22,300.00	$ 507,000.00
R-302	$ 26,000.00	$ 632,000.00
R-303	$ 30,900.00	$ 802,000.00
R-305	$ 34,200.00	$ 926,000.00
	Total Bare Module Cost =	$ 6,983,100.00

Using the total bare module cost of approximately $7 million from Capcost, we were able to determine the fixed capital investment of the optimized process to be about $10.5 million. The fixed capital investment for our process is the summation of the grass root costs for all of our equipment.

Finally, after recalculating our cash flow statement, we were able to get our final optimized NPV. Our final NPV was approximately $39 million. This is a major improvement when compared to the initial base case. The project would only take a little less than four years for the investment to be paid back. After determining the net present value, we broke down the yearly costs into specific categories, shown in Table A-15, and performed a sensitivity analysis to show how we were able to increase the net present value to about $39 million.

Table A-15. Pricing for Optimized Case per year

Total Revenue	$111,800,000
Raw Materials	$71,800,000
Cost of Operating Labor	$900,000
Cost of Utilities	$(100,000)

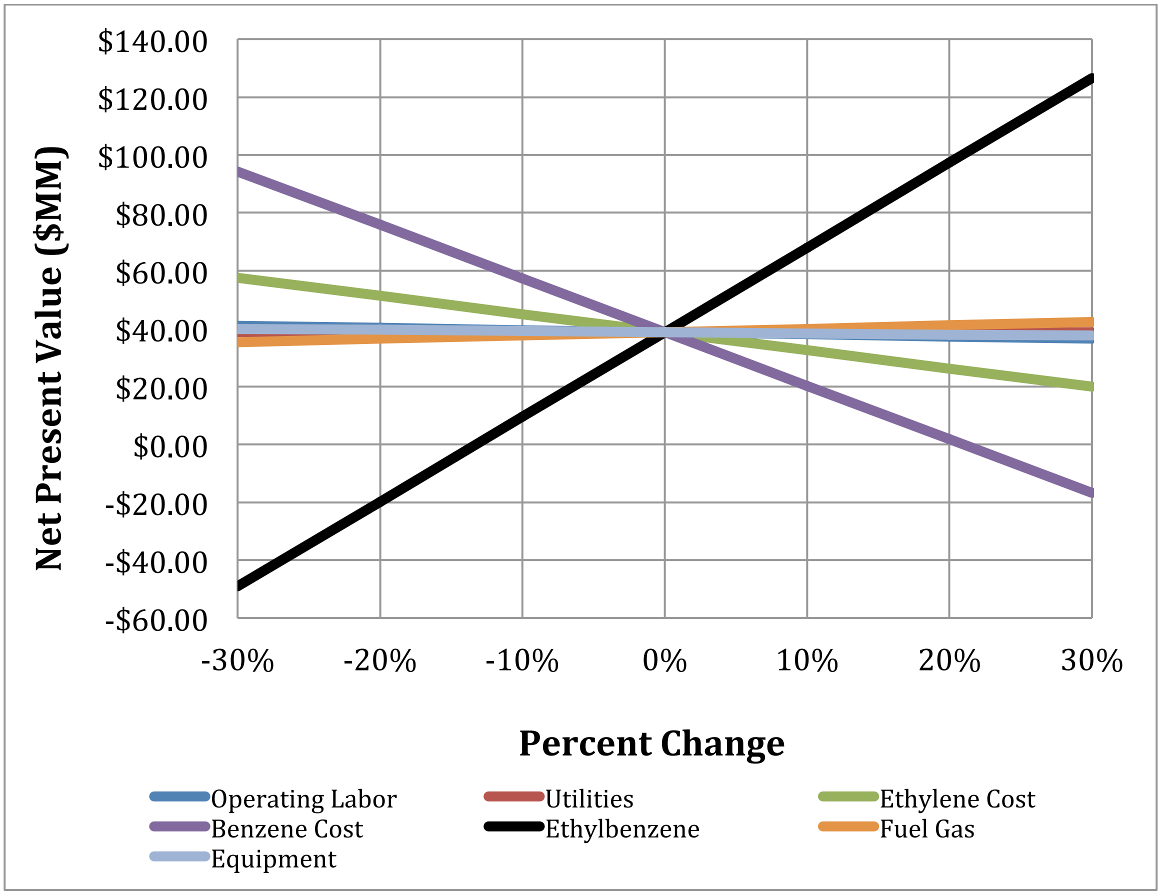


Figure A-11. Sensitivity Analysis for the Optimized Process

Compared to the base case, we decreased our cost of raw materials by approximately $14 million per year. As shown in the sensitivity analysis, the cost for our raw materials has one of the largest effects on the NPV. We also saw the total bare module cost for the optimized case increase but as shown in the sensitivity analysis, the equipment does not play much of a role in the NPV.

Conclusion

After working through this case study, we feel we have adequately optimized this facility to make this process a worthwhile investment. The base case presented to us had an NPV of about -$10.4 million. The first optimization steps we took were to investigate the two proposed changes as part of the initial case study. We determined that making both changes would increase the NPV the largest to approximately $31.9 million.

The next step we took was to determine the operating conditions for the reactor train. We determined the most economical choice is to run the reactors at high temperatures, high pressure, and a high ratio of benzene to ethylene. At these conditions, practically no DEB is produced. This allowed us to remove the second distillation column and therefore, the entire bottom recycle of DEB. In doing so, we were able to increase the NPV to $32.4 million. We then decided to investigate the possibility of putting a fourth reactor in the reactor train. Using four reactors increased the conversion of benzene and allowed us to use fewer raw materials. The effect of a fourth reactor increased the NPV of the process to $36.8 million. The last piece of equipment we optimized was the distillation tower. A few of the parameters we altered were the feed tray and the top tray pressure.

After all optimization changes were made, the process has an NPV of $39 million. This is a significant increase compared to the initial base case presented to us in the case study. The optimized process we have explained has increased the NPV from the base case by approximately $49.5 million. We advise that the optimized process we developed be followed in order to maximize profits. We also recommend determining the rate kinetics for higher ethylbenzene reactions in order to determine the optimum benzene to ethylene ratio into the reactors.

In the production of this facility, there are multiple safety aspects that need to be addressed. The largest concern deals with the temperature and pressure that the process operates at. Any equipment that is operating at high temperatures should be located out of reach of operators in order to minimize the chances of an operator to come in contact with the hot surface. In order to reduce the possibility of any accidents occurring from the high pressure, a pressure relief system should be installed. For example, if T-301 were to lose cooling water capacity, the tower could overpressure and have a loss of containment. A pressure relief valve would allow for the depressuring of this piece of equipment in a safe manner. One of the last concerns that needs to be considered is the terrorist proofing of the plant. Fences, guards, and other types of barriers need to be put in place to ensure the plant is operating safe.

Appendices

Appendix A-1: Nomenclature

$\eta = Efficiency$

$F_s = \ Vapor\ Factor\ \left(1.2 - 1.5\frac{m}{s}\left(\frac{kg}{m^3}\right)^{0.5}\right)$

$N_{min} = minimum\ number\ of\ stages$

$R_D = reflux\ ratio$

$m_{flow} = mass\ flow$

$n_{flow} = molar\ flow$

$MW = molecular\ weight$

$Density_{vap} = Density\ of\ the\ vapor$

$Density_{liq} = Density\ of\ the\ liquid$

Appendix A-2: Reactions and Kinetics

Reactions:

(1) $C_6H_6 + C_2H_4 \rightarrow C_6H_5C_2H_5$

(2) $C_6H_5C_2H_5 + C_2H_4 \rightarrow C_6H_4(C_2H_5)_2$

(3) $C_6H_4(C_2H_5)_2 + C_6H_6 \rightarrow 2C_6H_5C_2H_5$

(4) $C_6H_5CH_3 + 2C_2H_4 \rightarrow C_6H_5C_2H_5 + C_3H_6$

Component Key
$Benzene = C_6H_6$
$Ethylene = C_2H_4$
$EB = C_6H_5C_2H_5$
$DEB = C_6H_4(C_2H_5)_2$
$Toluene = C_6H_5CH_3$
$Propylene = C_3H_6$

Kinetics:

Reaction Kinetics are of the form:

$$-r_i = k_{o,i}\, e^{-\frac{E_i}{RT}}\, C_{ethlyene}^{a} C_{EB}^{b} C_{toluene}^{c} C_{benzene}^{d} C_{DEB}^{e}$$

where i is the reaction number above, and

Table 16. Comparison of the Kinetics for the Two Types of Catalyst

	Base Kinetics		**New Kinetics**						
i	**E_i (kcal/kmol)**	**$k_{o,i}$**	**E_i (kcal/kmol)**	**$k_{o,i}$**	**a**	**b**	**c**	**d**	**e**
1	22,500	$1.5\text{x}10^6$	22,500	$1.5\text{x}10^6$	1	0	0	1	0
2	22,500	$6.0\text{x}10^5$	22,500	$6.0\text{x}10^3$	1	1	0	0	0
3	25,000	$7.8\text{x}10^6$	25,000	$7.8\text{x}10^6$	0	0	0	1	1
4	20,000	$3.8\text{x}10^8$	20,000	$3.8\text{x}10^8$	2	0	1	0	0

Appendix A-3: Base Case Sensitivity Analysis

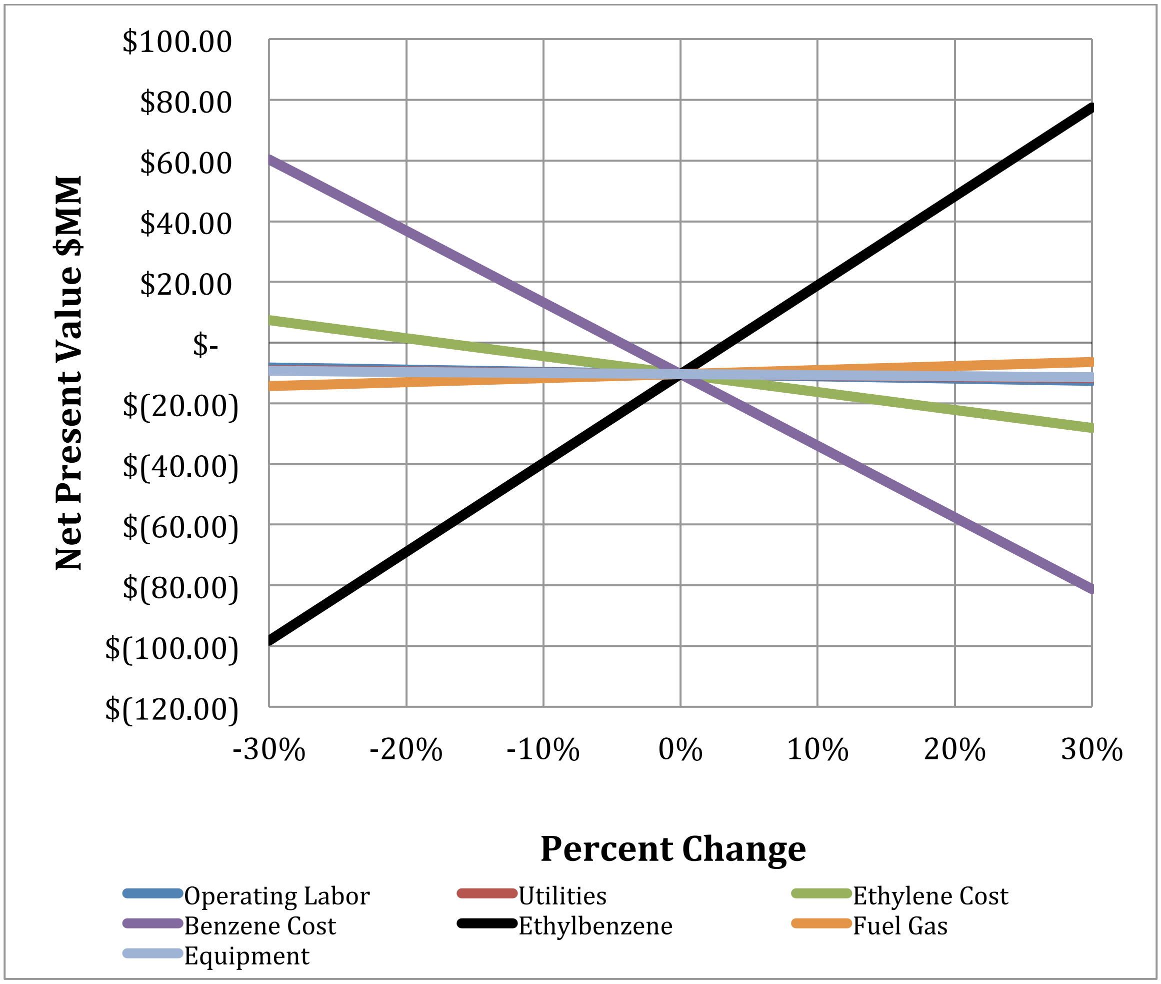


Figure A-12. Base Case Sensitivity Analysis

Appendix A-4: Equipment Calculations

Pump Sizing

Based upon heuristics, we determined the correct efficiency for each pump. Using Pro/II, we were able to determine the power for the pump. The actual power for the pump is given by:

$$Actual\ Power = \frac{Power}{\eta} \tag{4}$$

Tower Sizing

Using Pro/II, we determined the minimum number of stages from a shortcut column. As mentioned earlier in the report, we will use equation one to calculate the Actual number of stages.

$$Actual\ Stages = \frac{2\ N_{min}\ x\ 1.1}{\eta} \tag{1}$$

The 1.1 in equation 4 is to include a 10% safety factor. Based upon heuristics, there should be between 0.5 to 0.6 meters between each tray and a combined 3 meters of space split between the top and bottom for vapor disengagement and reboiler return. Using the actual number of stages and this heuristic, we are able to calculate the height of the tower.

$$Height\ (m) = 3\ + 0.55\ \ (Actual\ Stages - 1) \tag{5}$$

The last piece of information necessary for the distillation tower is the diameter.

$$V_{flow} = \frac{(1+R_D)\ m_{19}}{density_{vap}} \tag{6}$$

$$Velocity = \frac{F_S}{density_{vap}^{0.5}} \tag{7}$$

$$Diameter = 2\sqrt{\frac{V_{flow}}{\pi\ Velocity}} \tag{8}$$

This will need to be calculated four times. It needs to be done on the overhead vapor stream at the two values for F_S. Then it will need to be calculated based on the vapor in the bottom of the column at the two values for F_s.

Vessel Sizing

The heuristics used for this part of the calculations include a 50% liquid volume in each vessel. We also used a specific hold-up time dependent upon the function of each vessel.

$$V_{flow} = \frac{(MW)(n_{flow})}{density_{liquid}} \qquad (9)$$

$$Volume_{liquid} = (V_{flow})(holdup\ time) \qquad (10)$$

$$V_{vessel} = 2Volume_{liquid} \qquad (11)$$

$$Diameter = \sqrt[3]{\frac{4V_{vessel}}{3\pi}} \qquad (12)$$

$$Length = 3\ Diameter \qquad (13)$$

Reactor Sizing

Catalyst volume was obtained through a case study to determine the optimal volume. Length and diameter were determine from this.

$$D_{catalyst} = \sqrt[3]{\frac{4V_{catalyst}}{3\pi}} \qquad (14)$$

$$L_{catalyst} = 3\ D_{catalyst} \qquad (15)$$

The length of the reactor will be larger than the length given in equation 15. This is due to the fact that we need the vapor to spread out. The diameter will be the same as the diameter of the catalyst. We found the average open length in the reactors in the base case and used this same value to increase the length of catalyst to the actual length of the reactor. The average open space in the base case was 2.4 meters.

$$Length = 2.4\ L_{catalyst} \qquad (16)$$

Appendix A-5: Cash Flow Base Case

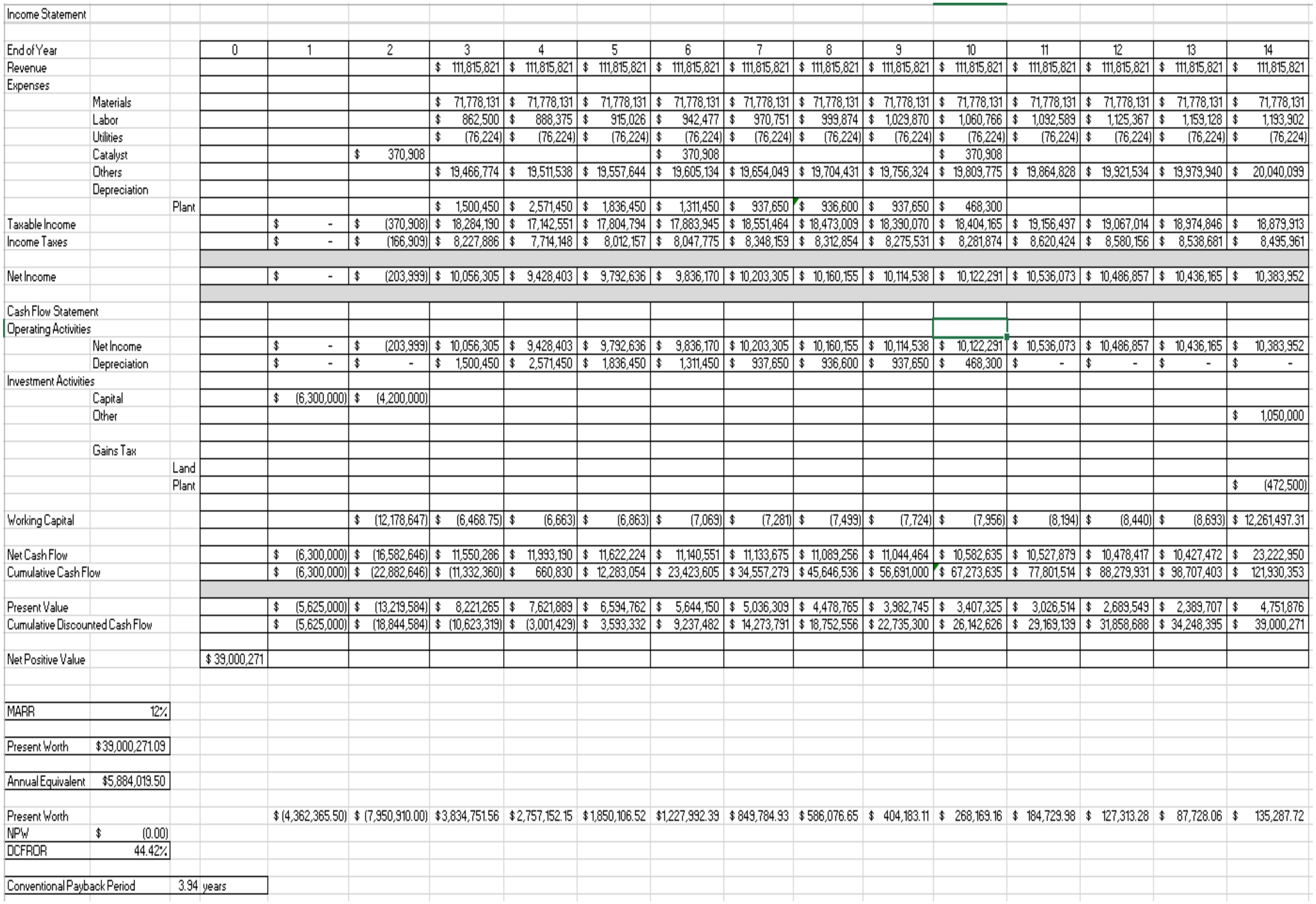
Located on next page.

Income Statement

End of Year			0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Revenue						$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564	$ 112,736,564
Expenses																	
	Materials					$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563	$ 85,838,563
	Labor					$ 862,500	$ 888,375	$ 915,026	$ 942,477	$ 970,751	$ 999,874	$ 1,029,870	$ 1,060,766	$ 1,092,589	$ 1,125,367	$ 1,159,128	$ 1,193,902
	Utilities					$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937	$ 1,324,937
	Catalyst				$ 276,012			$ 276,012			$ 276,012			$ 276,012			
	Others					$ 22,805,719	$ 22,850,483	$ 22,896,589	$ 22,944,079	$ 22,992,994	$ 23,043,376	$ 23,095,269	$ 23,148,719	$ 23,203,773	$ 23,260,479	$ 23,318,885	$ 23,379,044
	Depreciation																
		Plant				$ 1,368,982	$ 2,346,142	$ 1,675,542	$ 1,196,542	$ 855,494	$ 854,536	$ 855,494	$ 427,268				
Taxable Income				$ -	$ (276,012)	$ 535,863	$ (511,935)	$ (190,105)	$ 489,966	$ 753,825	$ 399,267	$ 592,431	$ 936,311	$ 1,000,690	$ 1,187,219	$ 1,095,051	$ 1,000,119
Income Taxes				$ -	$ (124,205)	$ 241,138	$ (230,371)	$ (85,547)	$ 220,485	$ 339,221	$ 179,670	$ 266,594	$ 421,340	$ 450,310	$ 534,248	$ 492,773	$ 450,053
Net Income				$ -	$ (151,807)	$ 294,725	$ (281,565)	$ (104,558)	$ 269,481	$ 414,604	$ 219,597	$ 325,837	$ 514,971	$ 550,379	$ 652,970	$ 602,278	$ 550,065
Cash Flow Statement																	
Operating Activities																	
	Net Income			$ -	$ (151,807)	$ 294,725	$ (281,565)	$ (104,558)	$ 269,481	$ 414,604	$ 219,597	$ 325,837	$ 514,971	$ 550,379	$ 652,970	$ 602,278	$ 550,065
	Depreciation			$ -	$ -	$ 1,368,982	$ 2,346,142	$ 1,675,542	$ 1,196,542	$ 855,494	$ 854,536	$ 855,494	$ 427,268	$ -	$ -	$ -	$ -
Investment Activities																	
	Capital			$ (5,748,000)	$ (3,832,000)												
	Other																$ 958,000
	Gains Tax																
		Land															
		Plant															$ (431,100)
Working Capital					$ (14,522,052)	$ (6,469)	$ (6,663)	$ (6,863)	$ (7,069)	$ (7,281)	$ (7,499)	$ (7,724)	$ (7,956)	$ (8,194)	$ (8,440)	$ (8,693)	$ 14,604,903
Net Cash Flow				$ (5,748,000)	$ (18,505,859)	$ 1,657,238	$ 2,057,915	$ 1,564,121	$ 1,458,955	$ 1,262,817	$ 1,066,634	$ 1,173,607	$ 934,283	$ 542,185	$ 644,530	$ 593,585	$ 15,681,868
Cumulative Cash Flow				$ (5,748,000)	$ (24,253,859)	$ (22,596,621)	$ (20,538,706)	$ (18,974,585)	$ (17,515,630)	$ (16,252,813)	$ (15,186,179)	$ (14,012,572)	$ (13,078,289)	$ (12,536,104)	$ (11,891,574)	$ (11,297,989)	$ 4,383,878
Present Value				$ (5,132,143)	$ (14,752,757)	$ 1,179,589	$ 1,307,842	$ 887,524	$ 739,152	$ 571,234	$ 430,795	$ 423,214	$ 300,814	$ 155,865	$ 165,435	$ 136,034	$ 3,208,821
Cumulative Discounted Cash Flow				$ (5,132,143)	$ (19,884,900)	$ (18,705,311)	$ (17,397,469)	$ (16,509,944)	$ (15,770,792)	$ (15,199,558)	$ (14,768,763)	$ (14,345,548)	$ (14,044,734)	$ (13,888,869)	$ (13,723,434)	$ (13,587,400)	$ (10,378,579)
Net Positive Value			$ (10,378,579)														
MARR	12%																
Present Worth	$ (10,378,578.97)																
Annual Equivalent	$ (1,565,829.14)																
Present Worth				$ (5,640,910.53)	$ (17,822,726.64)	$ 1,566,326.36	$ 1,908,785.71	$ 1,423,746.62	$ 1,303,276.38	$ 1,107,051.04	$ 917,645.34	$ 990,865.60	$ 774,110.56	$ 440,863.80	$ 514,319.03	$ 464,841.16	$ 12,051,805.57
NPV	$ (0.01)																
DCFROR	1.90%																
Conventional Payback Period		13.72	years														

Appendix A-6: Cash Flow Optimized Case

Located on next page.



Income Statement																	
End of Year			0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Revenue						$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821	$ 111,815,821
Expenses																	
	Materials					$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131	$ 71,778,131
	Labor					$ 862,500	$ 888,375	$ 915,026	$ 942,477	$ 970,751	$ 999,874	$ 1,029,870	$ 1,060,766	$ 1,092,589	$ 1,125,367	$ 1,159,128	$ 1,193,902
	Utilities					$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)	$ (76,224)
	Catalyst				$ 370,908				$ 370,908				$ 370,908				
	Others					$ 19,466,774	$ 19,511,538	$ 19,557,644	$ 19,605,134	$ 19,654,049	$ 19,704,431	$ 19,756,324	$ 19,809,775	$ 19,864,828	$ 19,921,534	$ 19,979,940	$ 20,040,099
	Depreciation																
		Plant				$ 1,500,450	$ 2,571,450	$ 1,836,450	$ 1,311,450	$ 937,650	$ 936,600	$ 937,650	$ 468,300				
Taxable Income				$ -	$ (370,908)	$ 18,284,190	$ 17,142,551	$ 17,804,794	$ 17,883,945	$ 18,551,464	$ 18,473,009	$ 18,390,070	$ 18,404,165	$ 19,156,497	$ 19,067,014	$ 18,974,846	$ 18,879,913
Income Taxes				$ -	$ (166,909)	$ 8,227,886	$ 7,714,148	$ 8,012,157	$ 8,047,775	$ 8,348,159	$ 8,312,854	$ 8,275,531	$ 8,281,874	$ 8,620,424	$ 8,580,156	$ 8,538,681	$ 8,495,961
Net Income				$ -	$ (203,999)	$ 10,056,305	$ 9,428,403	$ 9,792,636	$ 9,836,170	$ 10,203,305	$ 10,160,155	$ 10,114,538	$ 10,122,291	$ 10,536,073	$ 10,486,857	$ 10,436,165	$ 10,383,952
Cash Flow Statement																	
Operating Activities																	
	Net Income			$ -	$ (203,999)	$ 10,056,305	$ 9,428,403	$ 9,792,636	$ 9,836,170	$ 10,203,305	$ 10,160,155	$ 10,114,538	$ 10,122,291	$ 10,536,073	$ 10,486,857	$ 10,436,165	$ 10,383,952
	Depreciation			$ -	$ -	$ 1,500,450	$ 2,571,450	$ 1,836,450	$ 1,311,450	$ 937,650	$ 936,600	$ 937,650	$ 468,300	$ -	$ -	$ -	$ -
Investment Activities																	
	Capital			$ (6,300,000)	$ (4,200,000)												
	Other																$ 1,050,000
	Gains Tax																
		Land															
		Plant															$ (472,500)
Working Capital					$ (12,178,647)	$ (6,468.75)	$ (6,663)	$ (6,863)	$ (7,069)	$ (7,281)	$ (7,499)	$ (7,724)	$ (7,956)	$ (8,194)	$ (8,440)	$ (8,693)	$ 12,261,497.31
Net Cash Flow				$ (6,300,000)	$ (16,582,646)	$ 11,550,286	$ 11,993,190	$ 11,622,224	$ 11,140,551	$ 11,133,675	$ 11,089,256	$ 11,044,464	$ 10,582,635	$ 10,527,879	$ 10,478,417	$ 10,427,472	$ 23,222,950
Cumulative Cash Flow				$ (6,300,000)	$ (22,882,646)	$ (11,332,360)	$ 660,830	$ 12,283,054	$ 23,423,605	$ 34,557,279	$ 45,646,536	$ 56,691,000	$ 67,273,635	$ 77,801,514	$ 88,279,931	$ 98,707,403	$ 121,930,353
Present Value				$ (5,625,000)	$ (13,219,584)	$ 8,221,265	$ 7,621,889	$ 6,594,762	$ 5,644,150	$ 5,036,309	$ 4,478,765	$ 3,982,745	$ 3,407,325	$ 3,026,514	$ 2,689,549	$ 2,389,707	$ 4,751,876
Cumulative Discounted Cash Flow				$ (5,625,000)	$ (18,844,584)	$ (10,623,319)	$ (3,001,429)	$ 3,593,332	$ 9,237,482	$ 14,273,791	$ 18,752,556	$ 22,735,300	$ 26,142,626	$ 29,169,139	$ 31,858,688	$ 34,248,395	$ 39,000,271
Net Positive Value			$ 39,000,271														
MARR	12%																
Present Worth	$39,000,271.09																
Annual Equivalent	$5,884,019.50																
Present Worth				$ (4,362,365.50)	$ (7,950,910.00)	$3,834,751.56	$2,757,152.15	$1,850,106.52	$1,227,992.39	$ 849,784.93	$ 586,076.65	$ 404,183.11	$ 268,169.16	$ 184,729.98	$ 127,313.28	$ 87,728.06	$ 135,287.72
NPW	$ (0.00)																
DCFROR	44.42%																
Conventional Payback Period		3.94	years														

Appendix A-7: References

1. Turton, Richard. *Analysis, Synthesis, and Design of Chemical Processes*. Upper Saddle River, NJ: Prentice Hall PTR, 1998. Print.
2. Capcost Pricing Software. Turton
3. Perry, Robert H., Don W. Green, and James O. Maloney. *Perry's Chemical Engineers' Handbook*. New York: McGraw-Hill, 1984. Print.