

OPTIMIZATION OF AN ETHYLBENZENE PROCESS

by:  
Garrison Padgett Morgan

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:

---

Advisor: Dr. Adam E. Smith

---

Reader: Dr. John O'Haver

---

Reader: Dr. Clint Williford

© 2015  
Garrison Padgett Morgan  
ALL RIGHTS RESERVED

## ABSTRACT

Garrison Padgett Morgan: Process Optimization  
(Under the direction of Dr. Adam E. Smith)

In industry, chemical plants should be running at optimal performance in order to maximize profit. However, this is frequently not the case. Optimization is the process of improving an existing situation, device, or, in the case of chemical engineers, a chemical process. Furthermore, there are numerous strategies to optimize a chemical process, and it is up to the engineer to decide what to change in order to make the optimization worthwhile. Last semester, I was able to show my knowledge of optimization by applying changes to an existing ethylbenzene producing plant. I simulated the base case for this plant and created a cash flow statement that included revenue, raw materials cost, utilities, and other factors to generate a net present value of -\$11 million. Due to such a low net present value, I decided that drastic changes needed to be made in order to make the plant profitable. Using a sensitivity analysis to show what changes would help the most, I optimized the reactor chain section and the separation section of the plant. I will focus on the reactor chain section to show how I was able to optimize the plant in order to generate a new net present value of \$22.5 million.

## TABLE OF CONTENTS

LIST OF TABLES .....	v
LIST OF FIGURES .....	vi
INTRODUCTION .....	1
BACKGROUND ON OPTIMIZATION:	
TERMINOLOGY .....	2
STRATEGIES.....	3
TOPOLOGICAL AND PARAMETRIC OPTIMIZATION .....	7
EXAMPLE.....	11
CONCLUSION.....	18
REFERENCES .....	19
APPENDIX:	
PRODUCTION OF ETHYLBENZENE PROJECT .....	1
APPENDIX.....	44

## LIST OF TABLES

<b>Table 1:</b> Data Required for Base Case (in Addition to PFD and Flow Tables).....	3
<b>Table 2:</b> Characteristics of Easy and Difficult Optimization Problems.....	4
<b>Table 3:</b> Ranking of Contributions to the EAOC for DME Process.....	6

## LIST OF FIGURES

<b>Figure 1:</b> Process flow diagram of base case reactor section .....	12
<b>Figure 2.</b> Sensitivity analysis on base case net present value .....	12
<b>Figure 3.</b> Plot of conversion versus reactor temperature. The reactor temperature is representative of the entire reactor train, i.e. R-301 through R-303 .....	14
<b>Figure 4.</b> Plot of selectivity versus reactor temperature. As mentioned with Figure 3, reactor temperature is representative of the entire reactor train .....	14
<b>Figure 5.</b> Conversion to ethylbenzene in each reactor, as a function of reactor chain length.....	16
<b>Figure 6.</b> Process flow diagram of optimized reactor section of process .....	17

## **Introduction:**

There is no one correct way or strategy of optimizing each particular chemical process. It depends on what parameters are being optimized while satisfying the constraints of the process. The engineer must decide what can and cannot be changed in order to make the optimization profitable. The possibilities of variables to change in a chemical process are vast, so an engineer must focus on those with the most dramatic effect. In order to fully understand optimization, I will first discuss the basic terminology of optimization, such as design variables, objective functions, and optima. Then, different strategies that can be applied to a base case in order to help the engineer will be shown; for example, how to use top down and bottom up strategies and the use of Pareto analysis. Furthermore, there are two different types of optimization: topological and parametric. Both of these types of optimization play a crucial role in how a chemical process is manipulated in order to operate the chemical plant at full efficiency. Topological optimization deals with the topology or arrangement of process equipment, while parametric optimization deals with the operating variables for each given piece of equipment. After the background of optimization is discussed, I will show in an example of an ethylbenzene producing chemical plant how I have used this information in order to turn a base case into a more profitable optimized case. In conclusion, being able to optimize a chemical process is a fundamental part of how chemical engineers play a critical role in the chemical industry.

## **Background on Optimization:**

### Terminology:

When talking about optimization, decision variables, or design variables, are the independent parameters that an engineer may change. For example, the temperature of a reactor and the pressure in a separator are considered decision variables. The objective function is a mathematical function that reaches a maximum or minimum for certain values of the decision variables chosen. Maximizing or minimizing the objective function is how the process is optimized; profit and cost are two cases of what the objective function is trying to maximize or minimize, respectively. Additionally, any optimization problem is not limited to just one objective function, although the complexity of the problem will increase with added objective functions. As stated earlier, the variables that the engineer controls are the design variables. Constraints are limits on the values of these design variables or other product specifications. The two different types of constraints are equality, where a constraint is written as an equality involving two or more decision variables, and inequality, where a constraint is written as an inequality of one or more decision variables. An equality constraint reduces the dimensionality of the problem by eliminating the number of truly independent decision variables, while an inequality constraint applies boundaries to the problem. Another set of terminology used when talking about optimization is optima. Many times there will be local optima that are points where a small change in the decision variables in any direction will not improve the objective function. The best possible outcome of the objective function is a global optimum, where the objective function is best for all decision variables.



Strategies:

Now that the basic terminology for optimization has been explained, strategies to begin the process of optimization will be further explored. Optimization of any process all begins with a base case. There are no set rules on what a base case is or what it includes; it could be as simple as a basic flow sheet or an actual detailed chemical plant that needs to have modifications done to the previous design. The level of detail of a base case all depends on how much information is needed in order to obtain the objective function. Sizing and costing of equipment, material and energy balances, and utility costs are generally always included in the base-case analysis since they are decision variables that are involved in calculating the objective function. Data required for a base case can be seen below in Table 1, where the capital, operating, and material data can be seen separately.

**Table 1: Data Required for Base Case (in Addition to PFD and Flow Tables)**

<b>Capital</b>	<b>Operating</b>	<b>Material</b>
Installed Cost, price of each piece of equipment	Utility flowrates (each type)	Total cost for each raw material
	Utility targets	Value of purged or wasted material
Estimated credit for equipment used elsewhere in plant (for existing processes)	Utility costs on \$/GJ basis	Total product value
	Estimated uncertainties	Estimated uncertainties
Estimated uncertainties	Other operating costs	

Once a base case is obtained, an engineer is able to start strategizing on how the optimization will take place. But before any rigorous calculations and decisions are made, the problem-solving difficulty of the optimization must be estimated as “easy” or “difficult”. This may seem simple, however it helps plan out how much money, time, and resources will be needed in order to complete the problem. Examples of “easy” versus “difficult” problems can be seen and compared via Table 2 below.

**Table 2: Characteristics of Easy and Difficult Optimization Problems**

<b>Easy Problems</b>	<b>Difficult Problems</b>
Few decision variables	Many decision variables
Independent (uncorrelated) decision variables	Correlated decision variables
Discrete decision variables	Mixed discrete and continuous decision variables
Topological optimization first	Parametric optimization first
Single process units	Multiple, interrelated process units
Separate constraints for each decision variable	Constraints involving several decision variables
Constraints are obvious	Constraints are not obvious or become obvious only after the optimization has begun
Single objective	Multiple objectives
Objective function easy to quantify	Objective function difficult to quantify
Linear objective function	Highly nonlinear objective function
Smooth objective function	Kinked objective function
No local optima	Many deep, local optima

After the base case has been studied and characteristics estimated, one must decide how to go about the optimization. There are two different ways: top-down strategy and bottom-up strategy. Top-down strategy is taking a step back and analyzing the big picture of the process, then starting to look at the details of the problem. On the other hand, bottom-up strategy is the exact opposite, looking at the detailed calculations first, and then checking out the big picture of the process. Both strategies will essentially lead to the same result; it is just up to the preference of the engineer which strategy to use.

Optimization of a process all depends on what objective function is selected. If the objective function is poorly chosen, then all of the calculations and work may be wasted. The best way to choose the objective function is to make sure the extreme maximum or minimum is the most desired condition. The engineer is aiming to be able to achieve the global optimum of the objective function. Typical objective functions are in units of dollars, such as trying to maximize the net present value or minimize capital costs. However, there are objective functions that do not contain the units of dollars, such as trying to minimize the flow rate of a waste stream. Furthermore, there can be numerous objective functions per optimized case, for example trying to minimize the Equivalent Annual Operating Cost (EAOC) and minimize a waste stream. In these cases, the engineer needs to be able to analyze how much weight each objective function holds and if it is even feasible to reach the desired outcome. If not, then the objective functions need to be reselected or removed.

By analyzing the base case costs using a technique called *Pareto analysis*, one is able to determine what costs of the plant should be focused on and how key decision variables are chosen. Also known as the “80/20 Rule,” Pareto analysis is based on the

idea that eighty percent of the objective function is affected by only twenty percent of the contributing factors. In order to know what factors to examine, the contributing factors must be ranked in how much weight they pull in the overall objective function. To help visualize this technique, the operating costs and raw materials cost for a dimethyl ether (DME) process is shown in Table 3 below.

**Table 3: Ranking of Contributions to the EAOE for DME Process**

<b>Category</b>	<b>Contribution to EAOE (\$/y)</b>
Raw materials	11,215,000
Raw material (at 100% conversion) = \$11,185,000	
Target savings = \$30,300	
Medium-pressure steam	695,000
Towers and vessels	210,000
Heat exchangers	170,000
Pumps (including electricity)	160,000
Reactor	70,000
Cooling water	31,000
Wastewater treatment	1,000
<b>Total</b>	<b>12,552,000</b>

As can be seen from Table 3, the raw materials cost dominates all of the other costs in the list by contributing \$11,215,000/y to the total EAOE of \$12,552,000/y and is ranked first in the Pareto analysis. On the other hand, the wastewater treatment, which is ranked last, only contributes \$1,000/y to the EAOE and is not necessarily ignored but focus should be concentrated on another cost category. Ranking the costs of a process helps the engineer visualize what decision variables will make the most drastic change in the objective function and helps prevent wasted time trying to minimize a cost that will barely affect the optimization.

### Topological and Parametric Optimization:

Now that the terminology and fundamentals of optimizations have been discussed, one must be able to distinguish between the two types of optimization, topological and parametrical, and when to use each type. Topological optimization is concerned with the topology or layout of the process's equipment, while parametric optimization is dealing with the operating variables of the process such as pressures and temperatures of the process. In general, topological optimization is looked at first due to the fact that this type of optimizing has a lot of impact on the overall profit of the plant and that parametric optimization is easier once the topology of the process has been decided on.

When dealing with topological optimization, there are four major questions that need to be considered. The four questions should be addressed in the following order: can unwanted by-products be eliminated, can equipment be eliminated or rearranged, can alternative separation methods or reactor configurations be employed, and to what extent can heat integration be improved? First of all, the elimination of unwanted nonhazardous by-products or hazardous waste streams is extremely important to the overall optimization of a chemical process. When dealing with reactions, if there is not a 100% conversion of the reactants to the desired product(s), then the selectivity of the desired product might not be as high as wanted. The production of an unwanted by-product means more equipment has to be paid for and less product is produced, which in turn leads to less profit for the plant. It is vital to the design of the plant that the right catalyst and operating conditions are chosen in order to reduce the side reactions that occur. If the reaction results in the production of a hazardous waste stream, then treatment of this

stream must occur in order for the stream to be safe under environmental policies. This sometimes can be economically unfriendly and another reaction path must be chosen. A process engineer should always research alternative reaction paths, with varying conditions and reaction kinetics, to see how the different paths compare to one another and select the best overall technique to benefit the optimization.

The next question that should be analyzed deals with the elimination and rearrangement of equipment. The elimination of pieces of equipment has the potential to improve the overall economics of the plant by not only lowering the equipment cost but also eliminating associated utility costs for each piece of equipment. For example, if one is able to deem a distillation column unnecessary, then one not only does not have to pay for the column anymore but also the utility cost is lowered because boiler feed water and cooling water are not needed for that column. Additionally, the heat energy associated with the condenser and reboiler of the column is eliminated. However, sometimes the elimination of equipment upstream might overwhelm the equipment downstream by increasing the recycle stream flow rate or increasing utility costs, which would further increase the sizes of equipment needed downstream. The engineer must know what effect the elimination has on the process and whether or not to pursue it. The rearrangement of equipment can be changed based on guidelines for the sequence of pieces of equipment. For example, it is easier to pump a liquid rather than compress a gas. Rearranging equipment is frequently used when analyzing the separation section of a plant and heat integration so it will be further touched on in the next couple of sections.

In the early process of designing the chemical plant, separation methods should be examined to see which method would allow the best separation. Even though distillation

is the most common type of separation used in industry, other forms do exist depending on the properties being exploited. For example, centrifugation is used to concentrate a solid from a slurry, reverse osmosis is used to purify a liquid from a solution of dissolved solids, and adsorption is used to remove trace impurities from gas or liquid streams. Just as separation methods can be chosen, so can reactor configurations in a process. First, one must decide what type of reactor to use depending on the given reaction kinetics and thermodynamics, reactor parameters such as reactor volume and space time, and the amount of heat transfer being consumed or released by the reaction. The process engineer has the option to use a continuous-stirred tank reactor (CSTR), plug-flow reactor (PFR), or semi-batch reactor. Furthermore, after deciding which reactor to use, reactors can then be placed as a single unit, multiple units in series, multiple units in parallel, or multiple units in series and parallel to increase the conversion and selectivity of the desired product. Depending on what type of separation or reactor configuration is being used in the base case process, equipment might need to be eliminated or rearranged in order to substitute a better layout of the process in order to best optimize the plant.

The last question pertaining to topological optimization is whether or not heat integration can be improved. Throughout any chemical process, streams need to be heated or cooled in order for the desired outcomes to occur most efficiently. For example, a stream might need to be increased 200°C before entering the reactor so the conversion from reactant to product be greatly increased. Instead of using utilities to increase this stream to the correct temperature, maybe somewhere else in the plant there is a stream that can transfer the right amount of heat. The purpose of heat integration is to find

matches between heat being added and removed throughout the process and cut down on the need for additional utilities.

As stated earlier, parametric optimization deals with changing and optimizing different variables throughout the process. There are important variables that need to be analyzed carefully for every process. Reactor operating conditions play a strong role in determining the conversion of the reaction taking place. Temperature, pressure, concentration of reactants, amount of catalyst, and reactor length all can be manipulated to help obtain outcomes of the desired products. Purge ratios for recycle streams and reflux ratios in separating columns can be adjusted as well. A larger purge ratio may be needed to rid the process of unwanted chemicals, but also might increase the load on recycle stream equipment. The higher the reflux ratio, the fewer trays are needed for the column, and vice versa. All variables can be changed and manipulated by the process engineer within the given constraints, but the process engineer needs to know the direct consequences of changing anything and how it affects the objective function. Graphs of decision variables over a range of data can help determine where a maximum or minimum occurs and help choose the exact temperature, pressure, or reflux ratio needed for a certain process.

Single-variable optimization and multi-variable optimization are both types of parametric optimization. As the name suggests, single-variable optimization is changing one variable over a range and seeing how that change furthermore affects the chosen objective function. Multi-variable optimization is seeing how the changes of two or more variables over a range affect the chosen objective function. Both techniques of optimization are able to offer great data for optimizing a process, it just depends on how

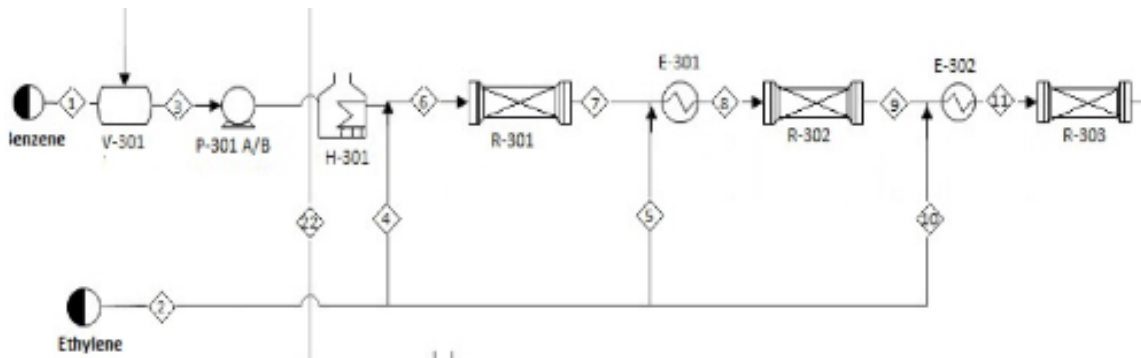


many variables one is trying to manipulate. By using multi-variable optimization, the data might be harder to collect due to all of the changing factors, but it will generate a better objective function outcome since it is incorporating more variables than single-variable optimization.

**Example:**

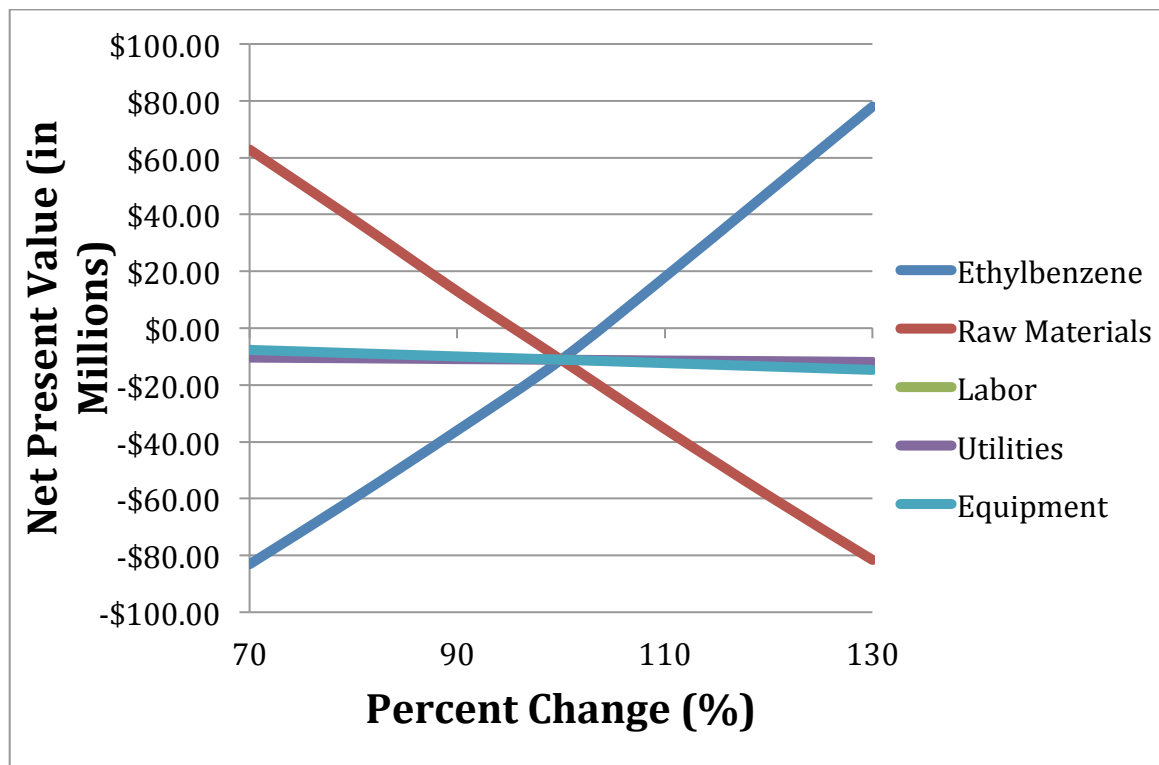
To conclude, I will talk about how I applied my knowledge of optimization to a base case of a plant that is producing 80,000 metric tonnes per year of 99.8% pure ethylbenzene. This criterion must be met no matter what is changed from the base case. Ethylbenzene is produced by the reaction of ethylene and benzene, however there are a series of unfavorable side reactions that occur. In order to minimize the amount of unwanted by-products, the feed to the reactor section of the plant is kept constant at an 8:1 ratio of benzene to ethylene. The incoming streams of ethylene and benzene are combined before being heated to 380°C in a fired heater. This combined stream is then fed to three different reactors in series. Due to the fact that the reactions taking place in each reactor are exothermic, the streams are cooled back down to 380°C by heat exchangers placed right before the reactors. After the reactor train, the stream is separated into a fuel gas stream and a stream that is sent to a series of distillation columns in order to achieve the desired product of ethylbenzene. Two separate recycle streams, one benzene rich and one diethylbenzene rich, come off the two distillation columns and return to the beginning of the process. After base case simulation and pricing was completed, my team determined that the overall net present value of the plant was -\$11

million. Optimization needed to take place in order for this chemical plant to be profitable.



**Figure 1.** Process flow diagram of base case reactor section

In order to know what changes would make the greatest impact, a sensitivity analysis was applied to the base case to see how incremental changes in certain parameters affected the net present value of the plant.



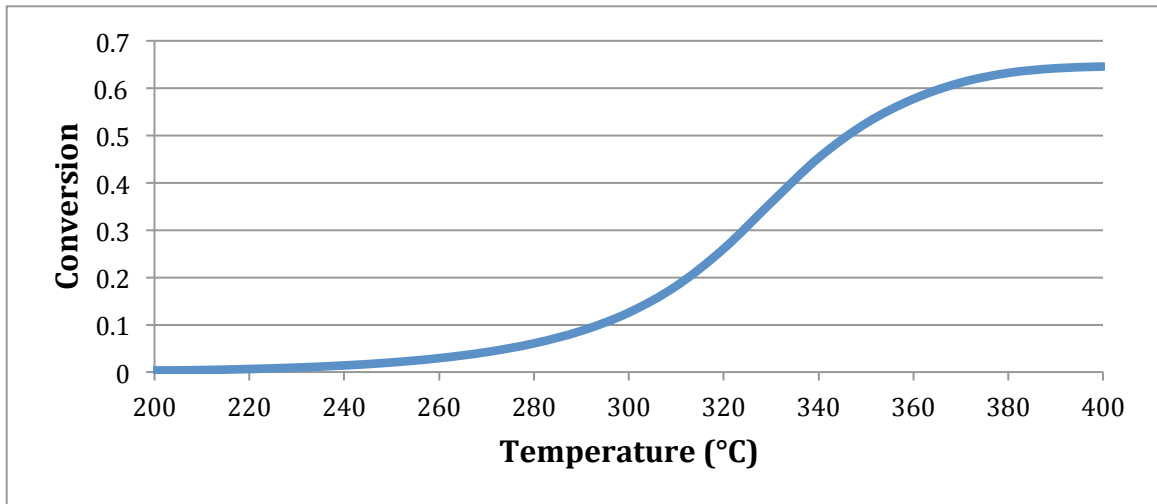
**Figure 2.** Sensitivity analysis on base case net present value.

From Figure 2, my team decided that the ethylbenzene and raw materials costs were the most sensitive to the net present value. However, since the ethylbenzene production had to stay at the design constraint of 80,000 metric tonnes produced per year, this category could not be changed. Even the slightest change of reducing raw materials cost could make the plant more profitable so my team chose to focus on decreasing the amount of raw materials purchased. We still sought to make changes to labor, utilities, and equipment costs but we knew what change to focus on in order to make the most profit.

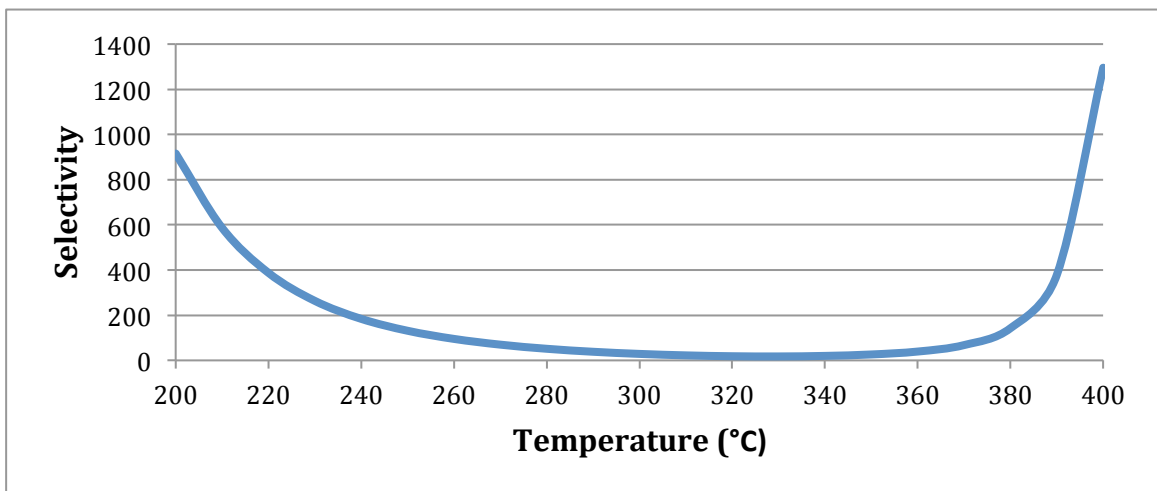
From the original base case problem statement, my team was given different options of cases to use. Change 1 involved changing the catalyst used in the reactors that saw an increase in price from \$5/kg to \$8/kg, an increase in life expectancy from 3 to 4 years, and an increase in bulk density from 1200 kg/m<sup>3</sup> to 1250 kg/m<sup>3</sup>. Change 2 suggested the use of benzene that contained 10% toluene for \$0.85/kg instead of the use of benzene that contained 3% toluene for \$1.04/kg. Change 3 was combining both Change 1 and Change 2. By simulation, we decided that Change 3 was the best route to take due to the fact that the net present value increased from -\$11 million to \$16.2 million.

Now that we knew the changes that would be used for our optimizing case, we were able to apply changes to the chemical process of the base case. As an example, I will focus on how we optimized the reactor section of the process and the effect on the net present value. Both parametric and topological optimizations were applied to this segment of the plant. First, the selectivity and conversion were analyzed over a range of

different temperatures in order to see the optimum temperature to produce the best conversion and selectivity. These two graphs can be seen below in Figure 3 and Figure 4.



**Figure 3.** Plot of conversion versus reactor temperature. The reactor temperature is representative of the entire reactor train, i.e. R-301 through R-303.

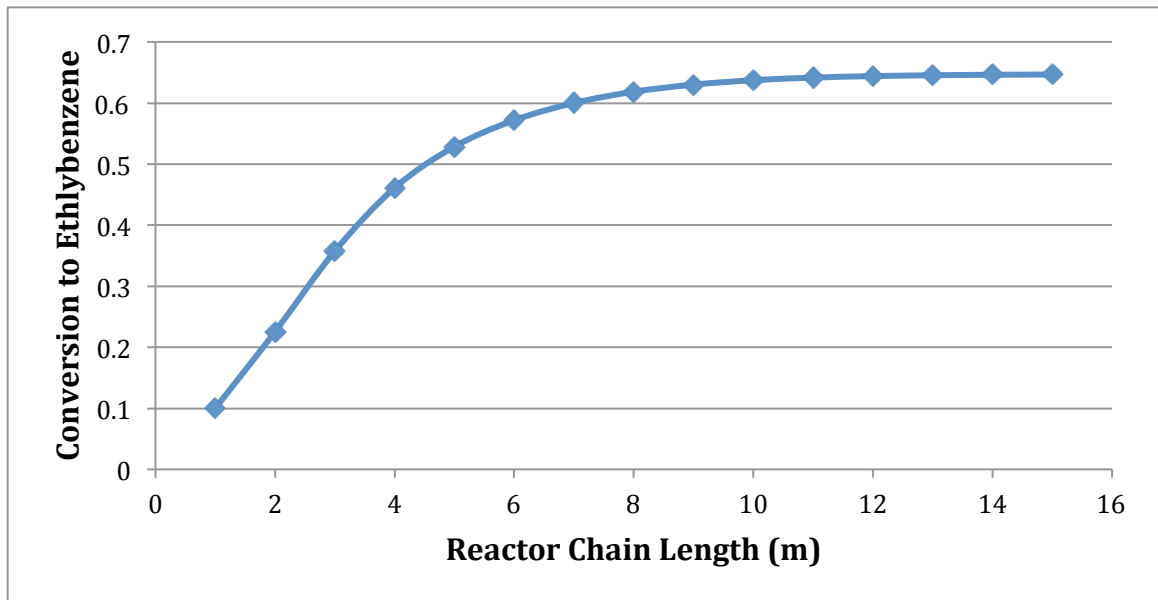


**Figure 4.** Plot of selectivity versus reactor temperature. As mentioned with Figure 3, reactor temperature is representative of the entire reactor train.

Through this use of parametric optimization, it was determined that the higher the temperature of the reactor train, the more ethylbenzene was being produced. After seeing the results of these single-variable optimizations, we decided to see how an increase in temperature through the reactor train would affect the conversion after the last reactor. By eliminating the heat exchangers E-301 and E-302 (the heat exchangers before the second and third reactors, respectively), the exothermic characteristic of the reaction increased the temperature throughout each reactor instead of keeping the incoming feed to each reactor at 380°C. This elimination of the two heat exchangers is an example of topological optimization. With the elimination of the heat exchangers, the reactors were now operating at temperatures over 400°C and would require stainless steel instead of much cheaper carbon steel material. One constraint that the reactors did have was that they were not allowed to be operated over 500°C due to the fact that it was the maximum allowable catalyst temperature. With this being said, the temperatures never exceeded 429°C so this temperature was operated well in the range of the catalyst constraint. However, the removal of the heat exchanges also saved money on utility and labor cost, while allowing a much larger production of ethylbenzene due to higher temperatures.

Another parametric optimization that we looked into was the reactor length of each reactor. By seeing how conversion changed with reactor length, we decided that the optimum length of each reactor should be 8 meters. Though this was a decrease of the reactor lengths from the base case, it proved that with the increased temperatures from the previously explained optimization this was the optimal length. Furthermore, it allowed the saving of more money on cost of materials due to decreased reactor length. As can be seen from Figure 5 below, the 8 meter reactor length does not actually provide

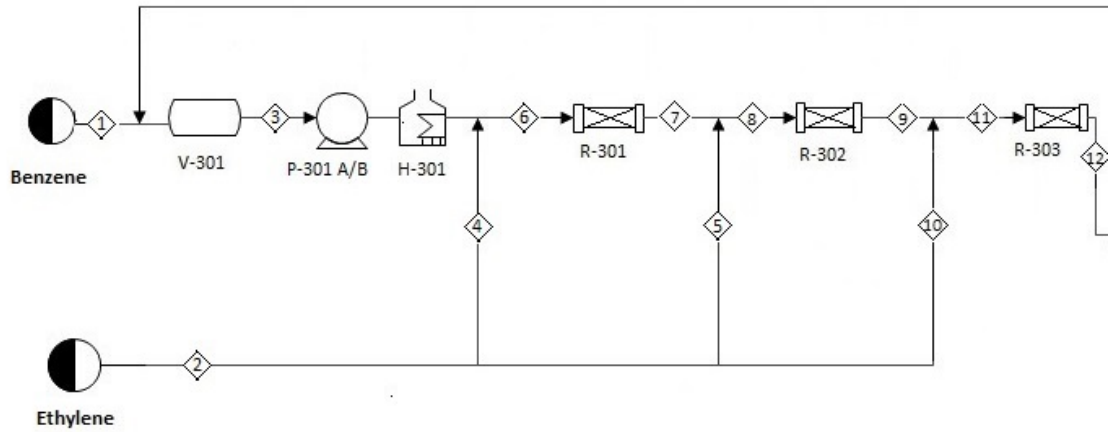
the greatest conversion to ethylbenzene at 0.62; the reactor chain length actually completely levels out at a conversion of 0.65 and a reactor length of 15 meters. By doing an economic analysis on the pricing of the reactors, we decided that a combined total cost of the 8 meter reactor section of \$1.6 million was much cheaper and worth the slightly lower conversion than the 15 meter reactor section of \$3 million.



**Figure 5.** Conversion to ethylbenzene in each reactor, as a function of reactor chain length.

These were the changes that were made to the reactor section that eliminated two heat exchanger costs, while increasing the overall amount of ethylbenzene produced. The optimized reactor section can be seen in Figure 6 below. The fact that the reactor section was able to convert more reactant to the desired product helped eliminate the need for the second distillation tower downstream, which further increased the net present value.

After optimization was completed, the net present value of the plant was \$22.5 million, a staggering increase from -\$11 million in the base case.



**Figure 6.** Process flow diagram of optimized reactor section of process.

**Conclusion:**

Optimization plays a role in any chemical plant, and with the proper use of its applications, any chemical plant in the industry can be running at optimal performance in order to reduce cost and maximize profit. Although there are multiple strategies of optimization, top down versus bottom up and topological versus parametric, the right application of these will provide changes to a chemical plant that will help it run more efficiently. As can be seen from my example of the optimization of the ethylbenzene producing plant, the first item that must be done is to analyze and create a base case cost. From there a sensitivity analysis is a great tool in order to see what factors will play the biggest role in how to make the biggest profit gain. Through my use of the different optimization strategies, my team was able to change a -\$11 million net present value to \$22.5 million. It can be tricky to know what and when to change and why to do it, but with the right skill set and practice, chemical engineers are vital in helping chemical plants reach their optimal performance.



**References:**

1. Turton, Richard, Richard C. Bailie, Wallace B. Whiting, Joseph A. Shaeiwitz, and Debangsu Bhattacharyya. "Chapter 14 Process Optimization." *Analysis, Synthesis, and Design of Chemical Processes*. Fourth ed. Upper Saddle River, NJ: Prentice Hall PTR, 2012. 451-97. Print.

# APPENDIX

# PRODUCTION OF ETHYLBENZENE

ChE 451 – Plant Design I

8<sup>th</sup> December 2014

Garrison Morgan, Chuck Rainey, Edna Rajan, and Ryan Smith

# Contents

Introduction.....	2
Results & Discussion .....	3
Base Case .....	3
Process Flow Diagram.....	4
Stream Flow Tables.....	6
Simulation Package .....	7
Equipment Sizing .....	8
Equipment Pricing.....	15
Operating Expenses.....	16
Net Present Value .....	19
Optimization.....	20
Sensitivity Analysis.....	20
Process Flow Diagram.....	24
Stream Tables .....	26
Process Description .....	27
Equipment.....	28
Equipment Summary Table.....	33
Cost Breakdown .....	35
Conclusion and Recommendations:.....	39
Nomenclature.....	41
Safety Aspect .....	43

## Introduction

It is proposed that an ethylbenzene plant that produces 80,000 metric tonnes per year of ethylbenzene be constructed. In the original scenario presented, or the *base case*, the process has a fixed feed ratio (8:1) of benzene to ethylene, a purity of 99.8% in the ethylbenzene product stream, and a fixed annual production as previously mentioned. Through a process concept diagram, a boxed analysis of streams flowing in and out of the process at large, we find that the production of EB can turn a profit:



**Figure 1.** Process concept diagram of the ethylbenzene process. Inlet streams are benzene and ethylene; product is ethylbenzene (3).

The diagram in Figure is based on the main reaction in the process, in which one mole of benzene (costing \$1.04 per kilogram) reacts with one mole of ethylene (\$0.72/kg) to form one mole of ethylbenzene (\$1.348/kg). On a kilogram-mole basis (i.e. 1000 gram-moles), the economic potential of the process is calculated as \$41.74 per kilomole of ethylbenzene.

With this in mind, the base case presents a problem: its *net present value*, or the total return on investment with interest rate considered, is a loss of \$11 million. The goal of our *optimization*, or the profit maximization of the investment, is to make changes to the process that meet the feed & product parameters but minimize the cost, and perhaps

to earn a profit. This has been performed through several changes that have been closely analyzed for performance and feasibility. Recommended changes involve a different reactor catalyst and a cheaper (but less concentrated) feed stream; from there, we create and analyze our own solutions.

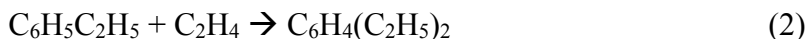
## Results & Discussion

### Base Case

The production of ethylbenzene emerges from a series of reactions, which begin with feeds of ethylene & benzene. The simple reaction is listed:



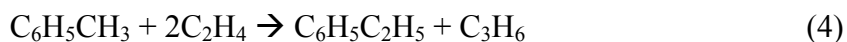
However, the ethylbenzene product reacts with ethylene to produce diethylbenzene:



Then, the diethylbenzene recycles with benzene to produce another yield of ethylbenzene:



Finally, the trace amount of toluene in the benzene feed reacts with the ethylene feed to form two products, including more ethylbenzene:

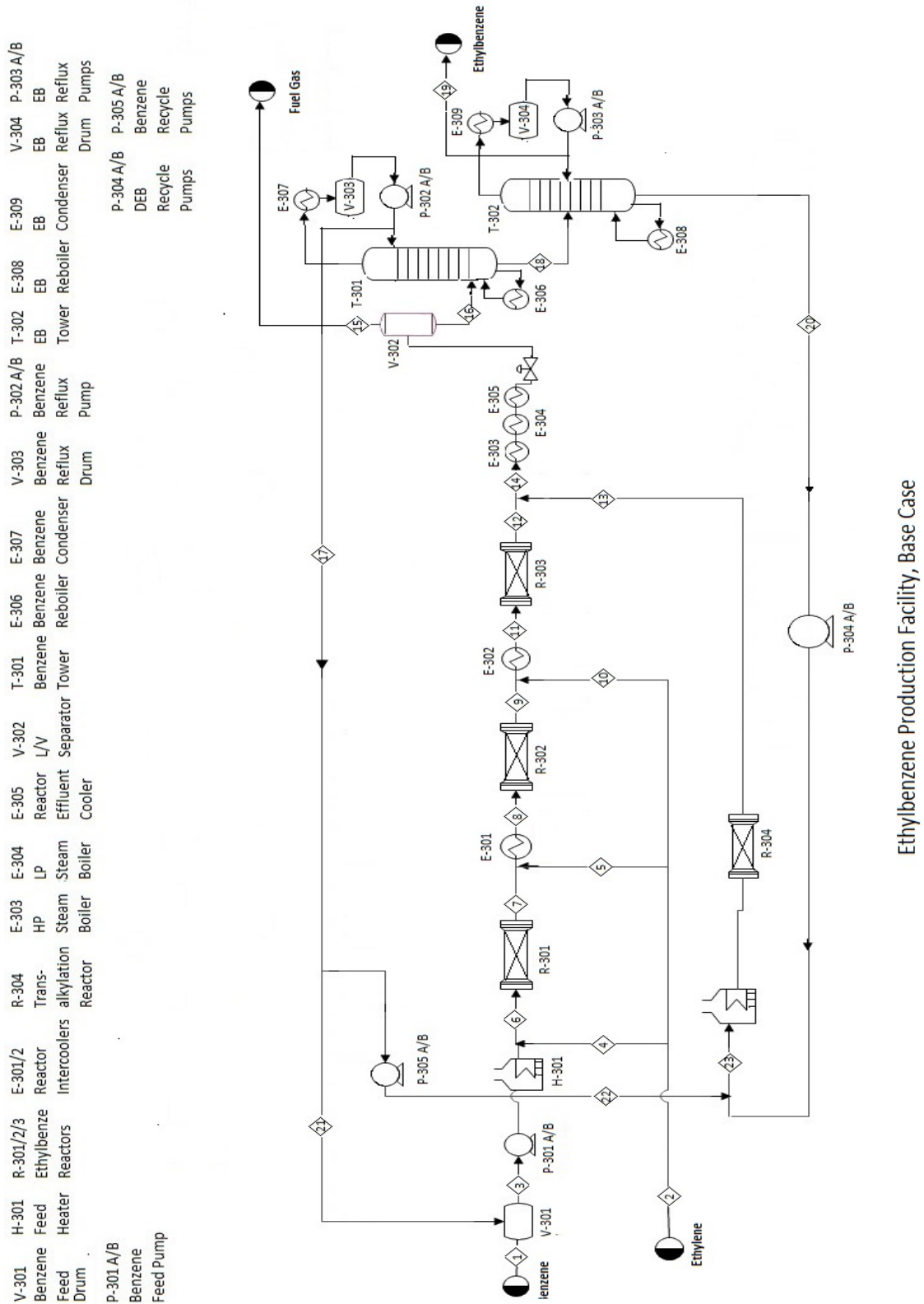


The benzene (97% benzene, 3% toluene) is prepared, using pumps, a vessel, and a fired heater, to react with three portions of the ethylene feed (93% ethylene, 7% ethane) in three reactors, each at 380°C. The product stream runs through three heat exchangers to cool to 80°C, after which the stream is pressurized (to 110 kilopascals) and a process

vessel splits the product into fuel gas, which will be consumed in another fired heater, and a stream that feeds into the first distillation column. This column, T-301, separates most of the benzene and lighter hydrocarbons from a stream of ethylbenzene and diethylbenzene. The light stream is recycled with the benzene feed; the bottom stream feeds into a second column, T-302. This tower separates the ethylbenzene, at 99.8% purity and with <2 parts per million diethylbenzene, from a DEB-heavy bottoms stream. The bottoms stream gets sent through a pump, back through the fired heater, and another reactor with the same kinetics as the first three. This product joins the stream from R-303 before approaching the series of heat exchangers.

The process flow diagram (PFD) for the base case plant is shown in the following page, with the *stream tables* after, or the data for each stream in the diagram:

# Process Flow Diagram



**Figure 1.** The process flow diagram for the base-case ethylbenzene production plant



## Stream Flow Tables

**Table 1.** Stream table for the streams featured in Figure 1. Some results are derived from Pro/II calculations.

Stream No.	1	2	3	4	5	6
Phase	Liquid	Vapor	Liquid	Vapor	Vapor	Vapor
Temperature (°C)	25	25	39.66	25	25	382.44
Pressure (kPa)	110	2000	110	2000	2000	2000
Total kg/h	7894.79	2875877	18168.73	862.76	1006.56	19049.49
Total kmol/h	100.53	102	233.30	30.60	35.70	263.60
Flowrates (kmol/h)						
Ethylene	0	94.86	0.07	28.46	33.20	28.52
Ethane	0	7.14	0.95	2.14	2.50	3.10
Propylene	0	0	1.18	0.00	0.00	1.18
Benzene	97.51	0	227.65	0.00	0.00	227.65
Toluene	3.02	0	3.02	0.00	0.00	3.02
Ethylbenzene	0	0	0.43	0.00	0.00	0.43
1,4-Diethylbenzene	0	0	0.00	0.00	0.00	0.00

Stream No.	13	14	15	16	17	18
Phase	Vapor	Vapor	Vapor	Liquid	Liquid	Liquid
Temperature (°C)	500.00	460.22	72.09	72.09	50.73	146.02
Pressure (kPa)	1988.00	1920.00	110.00	110.00	120.00	130.00
Total kg/h	5813.96	26876.56	1188.30	25688.26	13542.02	12155.68
Total kmol/h	65.83	309.98	21.07	288.91	174.70	114.35
Flowrates (kmol/h)						
Ethylene	0.00	0.77	0.68	0.09	0.09	0.00
Ethane	0.30	8.40	7.14	1.26	1.26	0.00
Propylene	0.37	4.56	3.02	1.55	1.55	0.00
Benzene	40.20	180.45	9.23	171.22	171.24	0.19
Toluene	0.00	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	24.95	115.07	1.00	114.07	0.57	113.43
1,4-Diethylbenzene	0.00	0.73	0.00	0.73	0.00	0.73

Stream No.	19	20	21	22	23
Phase	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	139.33	149.83	50.73	51.12	95.36
Pressure (kPa)	110.00	140.00	120.00	2000.00	2000.00
Total kg/h	9612.86	2454.83	10291.94	3250.09	5792.91
Total kmol/h	90.59	23.76	132.77	41.93	65.69
Flowrates (kmol/h)					
Ethylene	0.00	0.00	0.06	0.02	0.02
Ethane	0.00	0.00	0.95	0.30	0.30
Propylene	0.00	0.00	1.18	0.37	0.37
Benzene	0.18	0.01	130.14	41.10	41.11
Toluene	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	90.41	23.02	0.43	0.14	23.16
1,4-Diethylbenzene	0.00	0.73	0.00	0.00	0.73

## Simulation Package

In order to analyze this process, we were required to simulate it in a program called Pro/II. The program was able to perform mass & energy balance calculations based on our input, which included feed stream data, thermodynamics, reaction kinetics, equipment parameters, and process constraints (e.g. annual ethylbenzene output, 8:1 feed ratio, etc.). A vital component to the simulation was the selection of a thermodynamic package. Some of these were fairly popular equations of state: Soave-Redlich-Kwong (SRK), Peng-Robinson (PR) and the Wilson equation. For our process, we concluded that SRK-SIMSCI (SRKS) would fit best. The thermodynamic package guideline (attached) was used to determine the use of SRK-SIMSCI. Several factors led to our decision:

- There was no hydrogen or polar bonding
- The hydrocarbons were higher than C<sub>5</sub>
- H<sub>2</sub> was not present
- The temperatures in the reactors rose above 750 K

- The pressure was higher than 200 bar, but below 300 bar.

These factors led use to the use of the general SRK thermodynamic package. SRK-SIMSCI, a featured PRO/II package, introduced a new mixing rule to remove the error in the original Panagiotopoulos-Reid mixing rule. It also introduced an improved alpha correlation; i.e. it offered more accurate vapor pressure predictions than those of the original SRK equation. This package was designed to produce good results for aromatics hydrocarbons, which proved appropriate for this process.

### **Equipment Sizing**

Trial values for the feed streams were keyed into Pro/II, which then calculated the final stream data displayed in Table 1. Although Pro/II provided reliable balance calculations, the data had to be interpreted into further hand calculations. The size of the equipment was calculated based on stream information, temperature & pressure specifications, and other parameters either known or determined from Pro/II. The equipment, with approximate sizes determined, is displayed below, with calculation details following:

**Table 2.** Equipment summary for the base case process.

**Heat Exchangers**

<p><b>E-301</b>                      A = 54.1 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in tubes                      Q = 1,824 MJ/h                      Maximum pressure rating of 2200 kPa</p>	<p><b>E-302</b>                      A = 75.7 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in tubes                      Q = 2,671 MJ/h                      Maximum pressure rating of 2200 kPa</p>
<p><b>E-303</b>                      A = 433 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in tubes                      Q = 11,270 MJ/h                      Maximum pressure rating of 2200 kPa</p>	<p><b>E-304</b>                      A = 1200.8 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in tubes                      Q = 13,373 MJ/h                      Maximum pressure rating of 2200 kPa</p>
<p><b>E-305</b>                      A = 44.7 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in shell                      Q = 5,069 MJ/h                      Maximum pressure rating of 2200 kPa</p>	<p><b>E-306</b>                      A = 189 m<sup>2</sup>                      1-2 exchanger, fixed head, carbon steel                      Process stream in shell                      Q = 10,866 MJ/h                      Maximum pressure rating of 200 kPa</p>
<p><b>E-307</b>                      A = 151.9 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in shell                      Q = 9,657 MJ/h                      Maximum pressure rating of 200 kPa</p>	<p><b>E-308</b>                      A = 53.8 m<sup>2</sup>                      1-2 exchanger, fixed head, carbon steel                      Process stream in shell                      Q = 6,098 MJ/h                      Maximum pressure rating of 200 kPa</p>
<p><b>E-309</b>                      A = 18.6 m<sup>2</sup>                      1-2 exchanger, floating head, carbon steel                      Process stream in shell                      Q = 6,216 MJ/h                      Maximum pressure rating of 200 kPa</p>	

### Pumps

<p><b>P-301 A/B</b> Carbon steel – positive displacement Actual power = 14.5 kW Efficiency 75%</p>	<p><b>P-302 A/B</b> Carbon steel – centrifugal Actual power = Unknown Efficiency</p>
<p><b>P-303 A/B</b> Carbon steel – centrifugal Actual power = Unknown Efficiency unknown</p>	<p><b>P-304 A/B</b> Carbon steel – centrifugal Actual power = 1.9 kW Efficiency 80%</p>
<p><b>P-305 A/B</b> Carbon steel – positive displacement Actual power = 2.6 kW Efficiency 75%</p>	

### Fired Heater

<p><b>H-301</b> Required heat load = 25,429 MJ/h Design (maximum) heat load = 35,000 MJ/h 90% thermal efficiency Maximum pressure rating of 2,200 kPa</p>	
---	--

### Reactors

<p><b>R-301</b> Carbon steel, packed bed, ZSM-5 mol. sieve catalyst <math>V = 20\text{m}^3</math> 11m long, 1.72m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = <math>500^{\circ}\text{C}</math></p>	<p><b>R-302</b> Carbon steel, packed bed, ZSM-5 mol. sieve catalyst <math>V = 25\text{m}^3</math> 12m long, 1.85m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = <math>500^{\circ}\text{C}</math></p>
<p><b>R-303</b> Carbon steel, packed bed, ZSM-5 mol. sieve catalyst <math>V = 30\text{m}^3</math> 12m long, 1.97m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = <math>500^{\circ}\text{C}</math></p>	<p><b>R-304</b> Carbon steel, packed bed, ZSM-5 mol. sieve catalyst <math>V = 1.67\text{m}^3</math> 5m long, 0.95m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = <math>525^{\circ}\text{C}</math></p>

### Vessels

<b>V-301</b> 20.7m <sup>3</sup> Carbon steel Maximum operating pressure = 250 kPa Horizontal Height = 6.2m Diameter = 2.06m	<b>V-302</b> 4.9m <sup>3</sup> Carbon steel with stainless steel demister Maximum operating pressure = 250 kPa Vertical Height = 3.8m Diameter = 1.3m
<b>V-303</b> 8.05m <sup>3</sup> Carbon steel Maximum operating pressure = 300 kPa Horizontal L/D = 3	<b>V-304</b> 7.05 m <sup>3</sup> Carbon steel Maximum operating pressure = 300 kPa Horizontal L/D = 3

### Towers

<b>T-301</b> Carbon steel 23 sieve trays plus reboiler and total condenser 42% efficient trays Feed on tray 7 Reflux ratio = 0.5615 0.5 m tray spacing Column height = 14.5 m Diameter = 1.4m Maximum pressure rating of 300 kPa	<b>T-302</b> Carbon steel 24 sieve trays plus reboiler and total condenser 45% efficient trays Feed on tray 19 Reflux ratio = 0.5654 0.5 m tray spacing Column height = 15 m Diameter = 1.1 m Maximum pressure rating of 300 kPa
---	---

### *Heat Exchanger*

When we sized the heat exchangers, there were numerous variables to be considered—the presence or absence of a phase change, required heat duty, and the classification of utility being used. For heat exchangers involving a phase change, the areas of the latent and sensible sides were calculated, and then summed, to yield the total area of the heat exchanger. The main energy equation for the heat exchanger is presented:

$$Q = UAF_t\Delta T_{LM}. \quad (5)$$

The heat generated from the utility stream governed the overall heat transfer; this number varied depending on the utility used (i.e. boiler feed water, low pressure steam,

high pressure steam). The first calculation required was the mass flow rate of the utility, determined by:

$$Q = m\Delta H \quad (6)$$

$\Delta H$  was a product of steam table data;  $Q$  was interpreted from PRO/II. When the utility experienced the phase change (the case for E-301 to E-304), a technique called *zoned area analysis* was required. Under this condition, Equation 6 was used to determine heat transfer of sensible and latent exchanger zones,  $Q_{\text{sens}}$  and  $Q_{\text{latent}}$  (respectively). By use of a ratio,  $Q_{\text{latent}}:Q_{\text{total}}$ , the temperature difference between the latent and sensible side of the heat exchanger was found. Once this inside temperature was reached, we found  $\Delta T_{\text{LM}}$  for the sensible and latent sides of the exchanger. Equation 5 was used to find the area of each zone, using  $F_T$  values of 1 (for latent) and 0.9 (for sensible) and  $U = 60 \text{ W/m}^2\text{C}$  (from heuristics). Adding these zone areas yielded an overall heat transfer area. For E-305, the calculation required no phase change consideration, and thus was simpler.

The remaining exchangers were attached to the distillation columns, and acted as reboilers (E-306, E-308) or condensers (E-307, E-309), with no phase change. Equation 5 was again used to calculate area, with values of  $F_T = 1$ ,  $U = 850 \text{ W/m}^2\text{C}$  (condenser heuristic) or  $1140 \text{ W/m}^2\text{C}$  (reboiler heuristic), and  $Q$  read from PRO/II. A special condition applied for reboilers: a heuristic stated that the max flux in a reboiler was  $31.5 \text{ kW/m}^2$ . Therefore, if the calculated  $Q$  exceeded  $31.5 \text{ kW/m}^2$ , a different equation was used to calculate area:

$$A = Q/q_{\text{max}} \quad (7)$$

## *Pumps*

For the pumps, the “size” utilized is the required power:

$$W = \frac{1.67 \cdot \dot{V} \cdot \Delta P}{\eta} \quad (8)$$

Three variables are utilized in the calculation of power: volumetric flow rate,  $\dot{V}$ , efficiency,  $\eta$ , and pressure drop,  $\Delta P$ . An efficiency of 75% is given for P-301 and P-305, which fits the heuristic; P-304’s efficiency of 80% qualifies for the same reason.  $\Delta P$  for each pump was given in the stream data, and volumetric flowrate was interpreted from PRO/II.

## *Vessels*

The sizes of the process vessels, from Table 2, are reported by their length and diameter. On the recommendation of a heuristic, we sought an optimum height-to-diameter ratio, L/D, of 3. To determine an appropriate volume for each vessel, we used additional heuristics. For instance, when a vessel feeds into a furnace, 30 minutes are allowed to fill a drum until half-full. The flow rate leaving the drum was determined from the PRO/II simulation and multiplied by 30 minutes and 2 (since it is 30 minutes for a “half-full” drum). Then, from the calculated volume, the diameter and length were back calculated while keeping the L/D ratio equal to 3.

Another type of vessel, a reflux drum, was treated with a holdup time (i.e. time to fill the vessel half way) of 5 minutes. From there, the calculation was the same.

The sizing of the vessels on the two distillation columns was performed differently, since there were two products leaving the vessel: the reflux stream and the



exit stream. These flow rates, molecular weights, and densities of the streams exiting the vessel were read from the PRO/II simulation and used to calculate the total flow rate leaving the vessel, from which volume, length, and diameter could then be determined. Also of note: a holdup time of 10 minutes was used, since the vessel's products fed another tower.

### ***Tower***

Sizing the towers required many different variables to calculate the number of trays, height of the tower, and the diameter of the tower. Required for the calculations were: the reflux ratio for each tower, the minimum number of trays for each tower, and mass and volumetric flow rates for the distillate and bottoms streams of each tower. Finding these data required us to have our PRO/II simulation completely converged and required both shortcut and rigorous distillation columns for us to gather the required data. The shortcut columns provided us with the minimum reflux ratio and the minimum number of necessary trays, while the rigorous columns provided us with the necessary mass and volumetric flow rates.

For the reflux ratio:

$$R = (1.2 \rightarrow 1.5) * R_{min} \quad (9)$$

The number of operating trays:

$$N_{actual} = \frac{1.1 * 2 * N_{min}}{\eta} \quad (10)$$

The height of the tower:

$$H = 0.5 * N_{actual} + 3 \quad (11)$$

Average density of the distillate and bottoms streams:

$$\rho_i = \frac{\dot{m}_i}{\dot{V}_i} \quad (12)$$

Velocity range for each stream:

$$v_i = \frac{1.2 \rightarrow 1.5}{\rho_i} \quad (13)$$

Column diameter, top or bottom:

$$d_i = \frac{4 * \dot{V}_i^{0.5}}{\pi * v_i} \quad (14)$$

For both the top and the bottom of the tower, a range of diameters was found. We used the larger diameter to avoid issues such as pressure build-up, decreased flow rate, and a possible decrease in separation.

## **Equipment Pricing**

Using the sizes, required duty (if needed), and materials of construction listed in Table 2, we then priced the equipment using CAPCOST. The total cost of materials allowed us to determine the fixed capital investment required to construct the plant.

**Table 3.** Equipment prices and fixed capital investment for the base case process.

<b>Equipment</b>	<b>Type</b>	<b>BMC</b>
E-301	Heat Exchanger	\$ 106,000
E-302	Heat Exchanger	\$ 118,000
E-303	Heat Exchanger	\$ 328,000
E-304	Heat Exchanger	\$ 535,000
E-305	Heat Exchanger	\$ 97,400
E-306	Heat Exchanger	\$ 144,000
E-307	Heat Exchanger	\$ 147,000
E-308	Heat Exchanger	\$ 95,000
E-309	Heat Exchanger	\$ 87,400
H-301	Fired Heater	\$ 2,250,000
P-301 A/B	Pump	\$ 80,200
P-302 A/B	Pump	\$ 32,800
P-303 A/B	Pump	\$ 32,800
P-304 A/B	Pump	\$ 40,000
P-305 A/B	Pump	\$ 36,700
T-301	Tower	\$ 128,000
T-302	Tower	\$ 116,000
V-301	Vessel	\$ 76,700
V-302	Vessel	\$ 45,400
V-303	Vessel	\$ 42,400
V-304	Vessel	\$ 38,800
R-301	Reactor	\$ 213,000
R-302	Reactor	\$ 261,000
R-303	Reactor	\$ 297,000
R-304	Reactor	\$ 48,300

Total BMC	\$ 5,396,900
Grass Roots	\$ 8,581,071

## Operating Expenses

After the equipment cost was determined, the year-to-year operation costs had to be calculated. The utilities (essentially the energy required to run the equipment), the revenues & expenses associated with raw materials, and operating labor were configured and combined for this calculation.

**Table 4.** Yearly operating expenses for the base case.

ID	Description	Utility	Duty	Units	Efficiency	Actual Usage	Units	Annual Cost
E-301	Heat Exchanger	BFW	1830	MJ	100%	1.83	GJ	\$ (251,834)
E-302	Heat Exchanger	BFW	2700	MJ	100%	2.70	GJ	\$ (374,603)
E-303	Heat Exchanger	BFW	11300	MJ	100%	11.30	GJ	\$ (1,571,657)
E-304	Heat Exchanger	BFW	13400	MJ	100%	13.40	GJ	\$ (1,472,199)
E-305	Heat Exchanger	CW	5065	MJ	100%	5.07	GJ	\$ 14,921
E-306	Heat Exchanger	LPS	10860	MJ	100%	10.86	GJ	\$ 1,269,796
E-307	Heat Exchanger	CW	9657	MJ	100%	9.66	GJ	\$ 28,449
E-308	Heat Exchanger	HPS	6098	MJ	100%	6.10	GJ	\$ 898,232
E-309	Heat Exchanger	CW	6216	MJ	100%	6.22	GJ	\$ 18,312
H-301	Fired Heater	Fuel Oil (no. 2)	25429	MJ	90%	28.25	GJ	\$ 2,351,335
P-301	Pump	Electricity	14.5	kW	75%	19.33	KWh	\$ 9,654
P-302	Pump	Electricity	1	kW	75%	1.33	KWh	\$ 666
P-303	Pump	Electricity	1	kW	75%	1.33	KWh	\$ 666
P-304	Pump	Electricity	1.9	kW	80%	2.38	KWh	\$ 1,186
P-305	Pump	Electricity	2.57	kW	75%	3.43	KWh	\$ 1,711

Total Cost of Utilities per year	\$ 924,635
----------------------------------	------------

Chemical	Flowrate (kg/hr)	Cost (\$/kg)
Benzene	7894.8	1.04
Ethylene	2875.9	0.72

Total Cost of Raw Materials	\$ 85,560,479
-----------------------------	---------------

Chemical	Flowrate	Cost	\$/year
Fuel Gas	1190	0.514	\$ 5,090,235
Ethylbenzene	9613	1.348	\$ 107,839,172

Revenue	\$ 112,929,407
---------	----------------

Number of Nonparticulate Processing Steps	16
Number of Operators per Shift	3.15753
Number of Operators	15.0000

Cost of Operating Labor	\$ 862,500
-------------------------	------------

As illustrated by Table 4, our revenue was calculated by adding the income of ethylbenzene to that of the fuel gas, which yielded a total revenue of \$112.9 million per year. The expense of raw material was a sum of the ethylene feed cost, the benzene feed cost and the cost of the catalyst. The catalyst used in the base case cost \$5/kg and had an expected lifetime of 3 years. In order to determine the labor cost per year, the number of nonparticulate processing steps--compressors, towers, reactors, heaters, and exchangers--had to be determined. In the base case process, 16 pieces of equipment were considered nonparticulate. The number of operators was determined from the equation below:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (15)$$

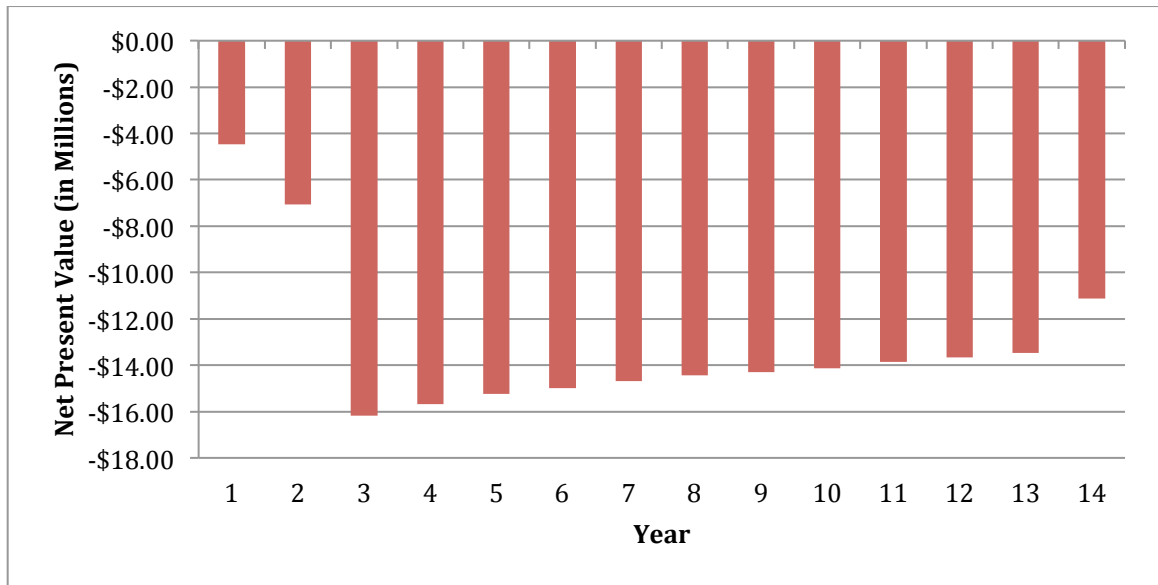
This equation yielded the value of roughly 3.2 operators per shift. Furthermore, by assuming annual wages of \$57,500 per operator, the total labor expense per year was calculated to be \$862,500; this cost increased by 3% each year. The expense of utilities was calculated by adding up the cost of electricity from the pumps, fuel gas from the fired heater, and cw, hps, or lps from the heat exchangers. The boiler feed water, however, produced a credit rather than a cost. The total expense for utilities per year came out to be \$924,635.

The capital investment, or the grass roots cost, was depreciated under the 7-year MACRS schedule. The construction period comprised the first two years of the project; the cost was distributed 60% in the first year and 40% in the second year. At the end of the project's lifetime, there was a salvage value of 10% FCI that could be recovered.

The working capital, the amount of capital required to start up the plant and finance the first few months of operation, was covered by 2 months' supply of raw materials plus 3 months of labor costs. This amount varied year to year due to the

increase of 3% of labor each year and the fluctuation of raw materials, which came from replacing the catalyst every 3 years.

The totals from each of these years, summed up over time, are illustrated by a cumulative cash flow diagram, which is shown as follows:



**Figure 2.** Discounted cash flow diagram. The net income/loss shown for each year equals the sum of that year's value & previous years' values. Production starts in year 3.

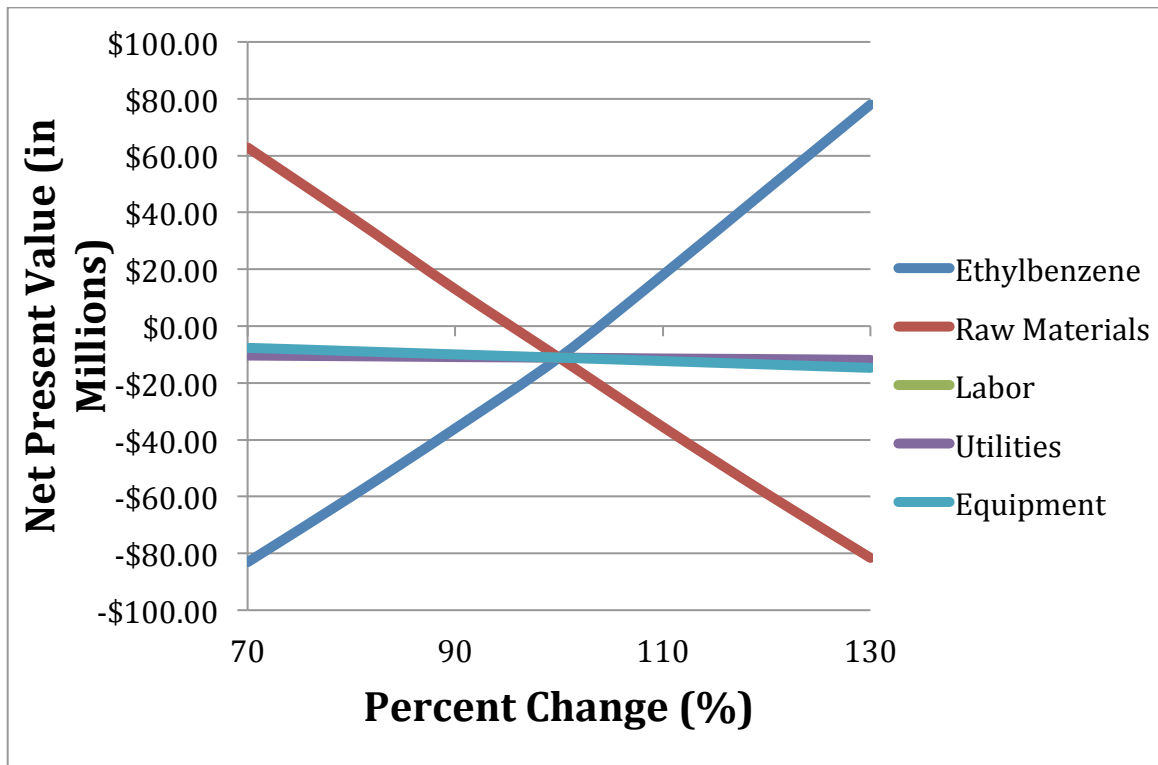
### Net Present Value

Using the time value of money, these annual values were combined to form a *net present value* (NPV), or today's financial benefit/burden resulting from an investment. The base case NPV was a loss of \$11 million. This would be an unsuccessful project investment. As can be seen in Figure 2, the conventional payback period was 13.8 out of 14 years. Due to this analysis of the base case, we decided that optimization of the plant needed to take place.

## Optimized Case

### Sensitivity Analysis

An immediate tool of investigation, a sensitivity analysis, was performed to illustrate how the NPV would change if certain parameters (i.e. raw materials, labor, etc.) were changed incrementally.



**Figure 3.** Sensitivity analysis on base case net present value.

From Figure 3, we gathered that ethylbenzene and the raw materials were the most sensitive parameters. This was expected, since our main revenue source was the ethylbenzene. As the design requirement was set at 80,000 tonnes/year of ethylbenzene, no changes could be made toward this parameter. It was found worthwhile, however, to investigate the raw materials: reducing this cost, even by a small percentage, could yield

a large increase in the net present value. We also sought to investigate labor, utilities, and equipment. Since labor and utilities proved intrinsic to equipment, we first took a look at the equipment. The base case utilized 25 pieces of equipment, a fact that was investigated to ensure the most cost-efficient amount and quality of equipment. Based on the equipment investigations, we could then alter the cost of labor and utilities.

### **Special Conditions**

Before optimizing the process equipment, we analyzed each piece of equipment for *special conditions*, or conditions of concern. These conditions were: high & low temperature, high & low pressure, non-stoichiometric feeds, large pressure increase (out-to-in ratio of three) within a compressor, a large log-mean temperature difference (above 100 degrees Celsius) across a heat exchanger, heaters with a higher process stream outlet temperature than supplied by the available steam, large pressure drops across process valves, and mixtures of streams with greatly different temperatures. These conditions could greatly increase operating and equipment costs, due to the need for special materials of construction, wasted energy, unnecessary duty, and extra separation costs; thus, we found it necessary to identify any special conditions found in our base-case equipment. The results are listed:



**Table 5.** Special conditions matrix, base case equipment.

Equipment	High Temp.	Low Temp.	High Pres.	Low Pres.	Non-Stoich. Feed	Comp	Exchanger	Heater	Valve	Mix
R-301	X		X		X					
R-302	X		X		X					
R-303	X		X		X					
R-304	X		X		X					
V-301			X							
V-302										
V-303										
V-304										
T-301										
T-302										
H-301								X		
E-301							X			X
E-302							X			X
E-303							X			
E-304							X			
E-305							X			
E-306							X			
E-307							X			
E-308							X			
E-309							X			
P-301										
P-302										
P-303										
P-304										
P-305										
PCV before V-302			X						X	

The matrix in Table 5 showed us the conditions that would either need to be justified or reconsidered through our optimization.

### **Analysis of Two Proposed Changes**

To begin our optimization, we were offered several changes to the process that we had to analyze; from there, we determined whether or not to use these options. Change 1 brought about a new catalyst, developed by our supplier, which would supposedly suppress the ethylation of ethylbenzene to give diethylbenzene. This new catalyst cost

\$8/kg, instead of \$5/kg, and had an expected lifetime of 4 years instead of 3. The new catalyst would also have a bulk density of 1250 kg/m<sup>3</sup>, instead of 1200 kg/m<sup>3</sup>. Both the void fraction and maximum operating temperatures stayed the same at 0.4 and 500°C, respectively. The next change, Change 2, was where we were given the opportunity to purchase a lower grade of benzene at \$0.85/kg, instead of \$1.04/kg. This would come at a cost, however: the lower grade of benzene contained 10 mol% toluene as opposed to the original 3 mol% toluene in the first benzene stream. The four options to choose for further optimization include implementing Change 1, Change 2, Change 1 and 2, or no change at all.

When the first change was made, an impact was immediately spotted: even though the new catalyst had a longer expected lifetime, the overall raw materials cost increased by roughly \$6 million. This change, by itself, decreased the net present value of the project to -\$12.1 million.

Next, we analyzed Change 2 by itself. The feed of benzene was changed to the lower grade valued at \$0.85/kg, which presented a \$6 million decrease in annual raw materials cost. In turn, the total raw materials cost equated to \$79.1 million (including the cost of the original catalyst). The resulting net present value came out to a value of \$14.5 million.

When implementing both Change 1 and Change 2 together, the overall net present value for the project increased further, now at \$16.2 million. Due to the results of the changes and the resulting net present values, our group decided to further optimize the process by choosing proposed Change 1 and Change 2. The lowered cost of the benzene feed clearly compensated for the decrease in purity. The drastic change in the net present

value made more sense in the context of Figure 2, which illustrates the raw materials' impact on the investment.

From there, we were able to create our own solutions to the problem. The process flow diagram for the optimized case is shown, followed by detailed explanations of our solutions:

# Process Flow Diagram

V-301	P-301 A/B	H-301	R-301/2/3	E-303	E-304	E-305	V-302	T-301	E-306	E-307	V-303	P-302 A/B
Benzene Feed Drum	Benzene Feed Pump	Feed Heater	Ethylbenzene Reactors	HP Steam Boiler	LP Steam Boiler	Reactor Effluent Cooler	L/V Separator	Benzene Tower	Benzene Condenser	Benzene Reboiler	Benzene Reflux Drum	Benzene Reflux Pump

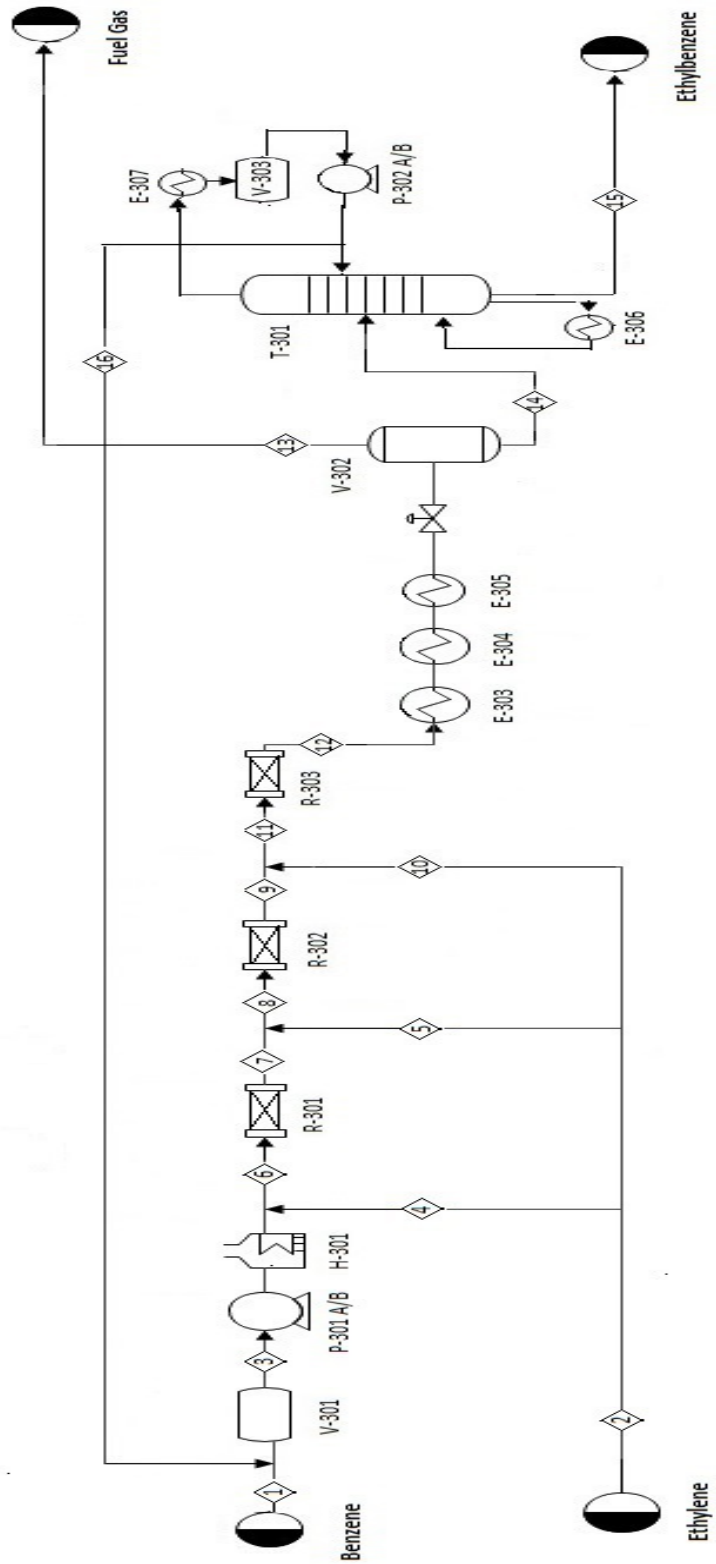


Figure 4. Optimized ethylbenzene process flow diagram.

## Stream Tables

**Table 6.** Data tables for the streams in Figure 4.

Stream No.	1	2	3	4	5	6
Phase	Liquid	Vapor	Liquid	Vapor	Vapor	Vapor
Temperature ( $^{\circ}\text{C}$ )	25.00	25.00	40.26	25.00	25.00	354.29
Pressure (kPa)	110.00	2000.00	110.00	2000.00	2000.00	2000.00
Total (kg/h)	8262.35	3084.52	20339.79	925.36	1079.58	21265.15
Total (kmol/h)	103.37	109.40	260.09	32.82	38.29	292.91
<b>Flowrates (kmol/h)</b>						
Ethylene	0.00	101.74	0.00	30.52	35.61	30.52
Ethane	0.00	7.66	0.83	2.30	2.68	3.13
Propylene	0.00	0.00	3.39	0.00	0.00	3.39
Benzene	93.04	0.00	244.33	0.00	0.00	244.33
Toluene	10.34	0.00	10.34	0.00	0.00	10.34
Ethylbenzene	0.00	0.00	1.19	0.00	0.00	1.19
1,4-Diethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00

Stream No.	7	8	9	10	11	12
Phase	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature ( $^{\circ}\text{C}$ )	398.48	380.11	448.70	25.00	429.41	495.27
Pressure (kPa)	1970.00	1970.00	1945.00	2000.00	1945.00	1920.00
Total (kg/h)	21265.15	22344.73	22344.73	1079.58	23424.31	23424.31
Total (kmol/h)	272.65	310.94	276.38	38.29	314.67	278.08
<b>Flowrates (kmol/h)</b>						
Ethylene	2.20	37.81	0.99	35.61	36.60	0.00
Ethane	3.13	5.81	5.81	2.68	8.49	8.49
Propylene	11.46	11.46	13.72	0.00	13.72	13.73
Benzene	232.15	232.15	199.84	0.00	199.84	163.27
Toluene	2.27	2.27	0.01	0.00	0.01	0.00
Ethylbenzene	21.44	21.44	56.00	0.00	56.00	92.59
1,4-Diethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00

Stream No.	13	14	15	16
Phase	Vapor	Liquid	Liquid	Liquid
Temperature (°C)	66.56	66.56	149.03	50.35
Pressure (kPa)	110.00	110.00	141.00	126.00
Total (kg/h)	1697.85	21726.46	9612.84	12113.62
Total (kmol/h)	30.75	247.34	90.59	156.75
<b>Flowrates (kmol/h)</b>				
Ethylene	0.00	0.00	0.00	0.00
Ethane	7.66	0.83	0.00	0.83
Propylene	10.34	3.39	0.00	3.39
Benzene	11.65	151.62	0.18	151.44
Toluene	0.00	0.00	0.00	0.00
Ethylbenzene	1.10	91.49	90.41	1.08
1,4-Diethylbenzene	0.00	0.00	0.00	0.00

## Process Description

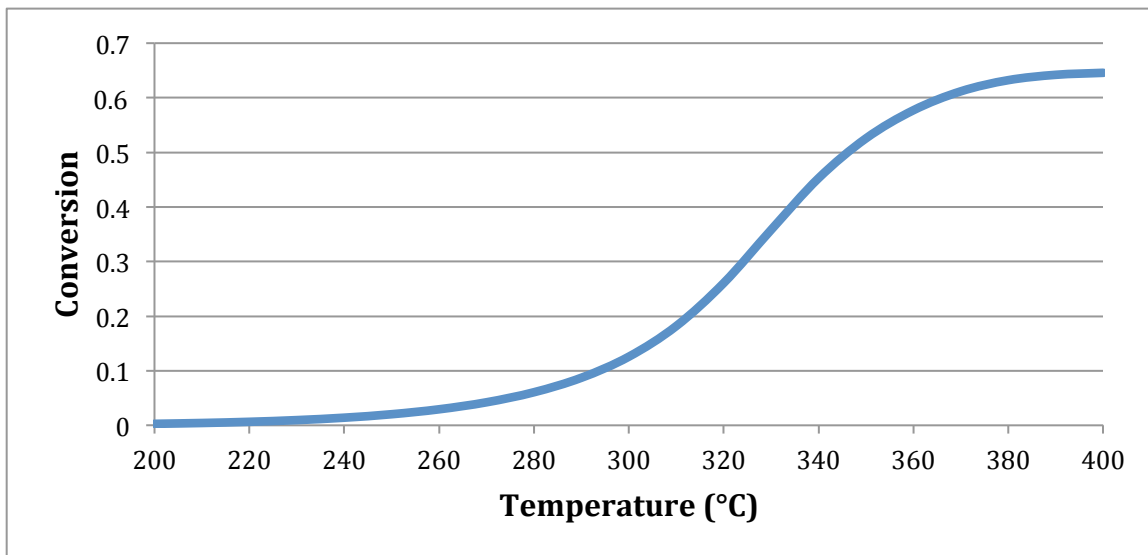
A refinery cut of benzene is fed from storage to an on-site process vessel (V-301) where it is mixed with recycled benzene. From V-301, it is pumped to 2,000 kPa and sent to a fired heater (H-301) to bring it to a reaction temperature (370°C). The preheated benzene is mixed with ethylene feed prior to entering a reactor system with three adiabatic packed-bed reactors (R-301 to R-303) with feed addition and cooling between stages. Reaction occurs in the gas phase and is exothermic. The stream from R-303 contains major products, by-products, unreacted benzene, and small amounts of unreacted ethylene and other non-condensable gases. The reactor effluent is cooled in two waste-heat boilers (E-301 and E-302) in which high- and low-pressure steams are generated, respectively. The process stream, now in two phases, gets sent to a trim cooler (E-303), where the stream is cooled to 80°C. After seeing a pressure decrease to 110 kPa in a valve, the stream is sent to V-302. This vessel separates the light gases from other products, and sends these gases overhead as a fuel gas, which will be consumed in the fired heater. The condensed liquid is then sent to a distillation tower, T-301, where the

unreacted benzene is separated and sent to the front end of the process. The bottoms product is composed of 99.8 mol% ethylbenzene and contains fewer than 2 ppm diethylbenzene.

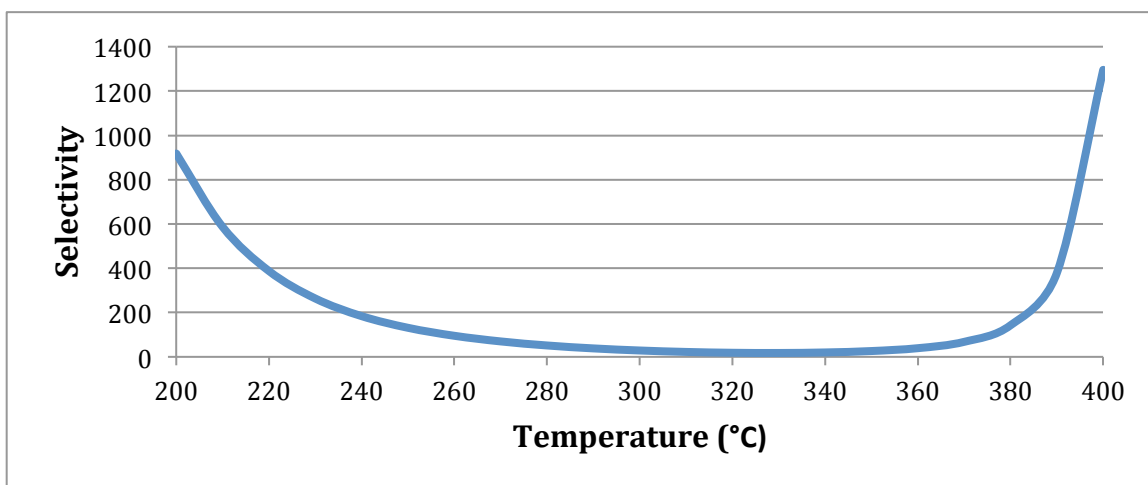
## **Equipment**

### ***Heat Exchanger***

First, it was found that we could remove heat exchangers E-301 and E-302. The function of E-301 and E-302 was to cool the feed to reactors R-302 and R-303, respectively, to 380 °C. This was done to maintain the reactor feeds at a uniform temperature. The various reactions that take place in these reactors are exothermic; therefore, the reactions release heat to the stream as a whole, adding natural heat to what would become the next reactor's feed. Thus, we investigated the effects of increasing reactor feed temperatures; from these changes, we observed effects on the conversion and selectivity of the reactions. When we removed E-301, the inlet temperature of R-302, stream 8, was at 380 °C and R-303, stream 11, was at 429 °C. We then were able to make plots of single-pass conversion and selectivity versus temperature, as shown in the following figures:



**Figure 5.** Plot of conversion versus reactor temperature. The reactor temperature is representative of the entire reactor train, i.e. R-301 through R-303.



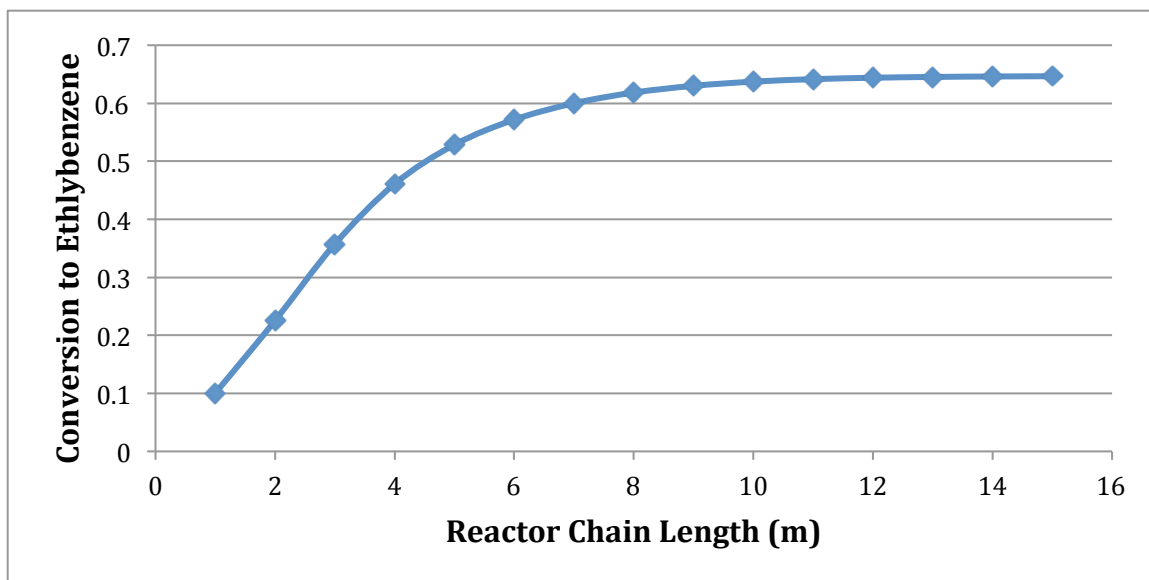
**Figure 6.** Plot of selectivity versus reactor temperature. As mentioned with Figure 3, reactor temperature is representative of the entire reactor train.



This proved the higher temperature favorable, as it increased the conversion and selectivity of ethylbenzene. As a result, the removal of E-301 and E-302 was beneficial to our process. By removing these two heat exchangers, we were able to save money on utilities and labor; we were required to change the material of two of the reactors, however. R-302 and R-303 would now be built with stainless steel, so the increased stress would not cause the equipment to fail.

### ***Reactor***

Another possible change in the reactor train arose from the consideration of each reactor's length. After analyzing the reactor chain as a whole, and seeing how conversion changed with reactor length, we decided on an optimum length of 8 meters for each reactor. This decision saw a decrease in reactor length from the base case, but a shorter reactor length proved necessary for increased reactor temperatures. These results are displayed in the figure below.



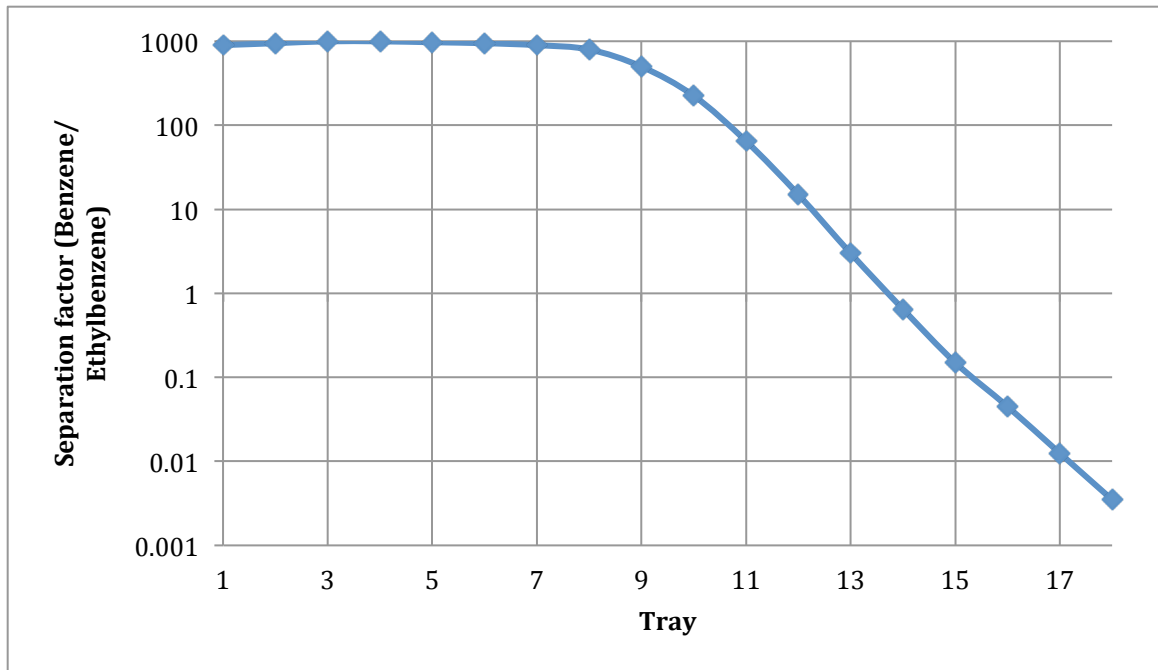
**Figure 7.** Conversion to ethylbenzene in each reactor, as a function of reactor chain length.

### ***Tower***

We also investigated of the elimination of the second distillation tower, T-302, and the recycled bottoms stream associated with it. The intention was to reduce the heat duty of the fired heater, H-301, eliminate one reactor, R-304, and eliminate two pumps, P-304 and P-305. When we realized that a very small amount of diethylbenzene ran in the recycle stream, compared to the rest of the system, we concluded that the recycle stream was a waste of resources. After we eliminated the second tower, the recycle stream, and all of the equipment associated with that tower and stream, we had to make minor adjustments to keep the ethylbenzene product stream within the required specifications. Once these requirements were met, the changes ended up handily decreasing our net present value, mostly through the change in utility cost. We were able to eliminate the \$100 thousand dollar bare module cost of the tower, several hundred thousand dollars due to the decreased duty of the fired heater, the ~\$100 thousand bare module cost attached to

reactor R-304, and the \$30 thousand cost attached to pumps P-304 and P-305 each. The end result was a decreased bare module cost of around \$500 thousand dollars which, when combined with utility costs and a decrease in labor, yielded massive cash savings.

Finally, after elimination of the second distillation column, we needed to ensure that the remaining distillation column could separate the tower feed (stream 16) in an efficient manner. Reading from Figure 4, Stream 16 has a rate of 246.5 kmol/hr, comprising 90.7 kmol/hr ethylbenzene and 151.6 kmol/hr benzene. After the separation occurred in the distillation tower, there was a recovery of 99.7% ethylbenzene in the bottom product stream and a recovery of 99.9% benzene in the top recycle stream. When analyzing changes in the separation factor with respect to the tower trays, we decided the best separation would come with a feed tray location of 7. This was the farthest tray from the reboiler that would not decrease the separation factor. The results are shown in the figure below.



**Figure 8.** Plot of the separation factor (i.e. ability to separate benzene from ethylbenzene) vs. feed tray location.

Our main goal in optimizing the process, of course, was to maximize the bottom line: the net present value. With our proposed changes came alterations to the equipment sizes, which turned into a new fixed capital investment. The optimized equipment summary table and the cost breakdown are to follow.

## Equipment Summary Table

Table 7. Revised equipment summary.

### Heat Exchangers

<p><b>E-303</b>  A = 407 m<sup>2</sup>  1-2 exchanger, floating head, carbon steel  Q = 11,854 MJ/h  Maximum pressure rating of 2,200 kPa</p>	<p><b>E-304</b>  A = 1040 m<sup>2</sup>  1-2 exchanger, fixed head, carbon steel  Q = 11,618 MJ/h  Maximum pressure rating of 2,200 kPa</p>
<p><b>E-305</b>  A = 39 m<sup>2</sup>  1-2 exchanger, floating head, carbon steel  Q = 4,443 MJ/h  Maximum pressure rating of 2,200 kPa</p>	<p><b>E-306</b>  A = 143 m<sup>2</sup>  1-2 exchanger, fixed head, carbon steel  Q = 10,218 MJ/h  Maximum pressure rating of 200 kPa</p>
<p><b>E-307</b>  A = 227 m<sup>2</sup>  1-2 exchanger, floating head, carbon steel  Q = 9,041 MJ/h  Maximum pressure rating of 200 kPa</p>	

### Pumps

<p><b>P-301 A/B</b>  Carbon steel – positive displacement  Actual power = 16.2 kW  Efficiency = 75%</p>	<p><b>P-302 A/B</b>  Carbon steel – centrifugal  Actual power = unknown  Efficiency unknown</p>
---	---

### Fired Heater

<p><b>H-301</b>  Required heat load = 19,400 MJ/h  Design (maximum) heat load = 35,000 MJ/h  90% thermal efficiency  Maximum pressure rating of 2,200 kPa</p>	
---	--

### Towers

<p><b>T-301</b>  Carbon steel  22 sieve trays plus reboiler and total condenser  75% efficient trays  Feed on tray 7  Reflux ratio = 0.51995  0.5 m tray spacing  Column height = 14 m  Diameter = 1.3 m  Maximum pressure rating of 300 kPa</p>	
--	--

**Reactors**

<p><b>R-301</b> Carbon steel packed bed, ZSM-5 mol. sieve catalyst V = 24 m<sup>3</sup> 10.3 m long, 1.72 m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C</p>	<p><b>R-302</b> Stainless steel packed bed, ZSM-5 mol. sieve catalyst V = 29 m<sup>3</sup> 10.7 m long, 1.85 m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C</p>
<p><b>R-303</b> Stainless steel packed bed, ZSM-5 mol. sieve catalyst V = 33 m<sup>3</sup> 10.7 m long, 1.97 m diameter Maximum pressure rating of 2,200 kPa Maximum allowable catalyst temperature = 500°C</p>	

**Vessels**

<p><b>V-301</b> 23 m<sup>3</sup> Carbon steel Maximum operating pressure = 250 kPa Horizontal Height = 6.43 m Diameter = 2.14 m</p>	<p><b>V-302</b> 4 m<sup>3</sup> Carbon steel Maximum operating pressure = 250 kPa Vertical Height = 3.6 m Diameter = 1.2 m</p>
<p><b>V-303</b> 7.5 m<sup>3</sup> Carbon steel Maximum operating pressure = 300 kPa Horizontal L/D = 3</p>	

## Cost Breakdown

**Table 8.** Equipment costs and fixed capital investment, optimized case.

Equipment	Type	BMC
E-303	Heat Exchanger	\$ 312,000
E-304	Heat Exchanger	\$ 492,000
E-305	Heat Exchanger	\$ 95,000
E-306	Heat Exchanger	\$ 128,000
E-307	Heat Exchanger	\$ 187,000
H-301	Fired Heater	\$ 2,030,000
P-301 A/B	Pump	\$ 84,500
P-302 A/B	Pump	\$ 32,800
T-301	Tower	\$ 138,000
V-301	Vessel	\$ 83,300
V-302	Vessel	\$ 40,700
V-303	Vessel	\$ 40,400
R-301	Reactor	\$ 204,000
R-302	Reactor	\$ 662,000
R-303	Reactor	\$ 757,000
Total BMC		\$ 5,286,700
Grass Roots		\$ 8,405,853

As Table 8 shows, the equipment cost did not decrease by a large amount between cases (refer to Table 3). Due to the fact that equipment was eliminated from the process, one would think that the equipment cost would drop sufficiently. The absence of certain pieces of equipment, along with the newly stainless steel-clad reactors, increased the load on the pieces remaining, which increased heat duties. As a result of higher duty, the equipment sizes increased, thus raising equipment prices once more. The sensitivity analysis in Figure 2 justifies this change: the equipment cost does not play much of a role in changing the net present value. There was another aspect of the plant, however, that greatly impacted the consequences of investment.

**Table 9.** Yearly operating costs for the optimized case.

ID	Description	Utility	Duty	Units	Efficiency	Actual Usage	Units	Annual Cost
E-303	Heat Exchanger	BFW	11854	MJ	100%	11.85	GJ	\$ (1,653,261)
E-304	Heat Exchanger	BFW	11618	MJ	100%	11.62	GJ	\$ (1,263,840)
E-305	Heat Exchanger	CW	4442	MJ	100%	4.44	GJ	\$ 13,086
E-306	Heat Exchanger	LPS	10217	MJ	100%	10.22	GJ	\$ 1,194,614
E-307	Heat Exchanger	CW	9040.7	MJ	100%	9.04	GJ	\$ 26,634
H-301	Fired Heater	Fuel Oil (no. 2)	19376	MJ	90%	21.53	GJ	\$1,791,634.13
P-301	Pump	Electricity	16.21	kW	75%	21.61	KWh	\$ 10,792
P-302	Pump	Electricity	1	kW	75%	1.33	KWh	\$ 666

Cost of Utilities	\$ 120,325
-------------------	------------

Chemical	Flowrate (kg/hr)	Cost (\$/kg)
Benzene	8223	0.85
Ethylene	3084	0.72

Total Cost of Raw Materials	\$ 76,645,870
-----------------------------	---------------

Chemical	Flowrate (kg/hr)	Cost (\$/yr)	\$/year
Fuel Gas	1693	0.514	\$ 7,241,821
Ethylbenzene	9613	1.348	\$107,839,172

Revenue	\$ 115,080,993
---------	----------------

<b>Number of Nonparticulate Processing Steps</b>	10
<b>Number of Operators per Shift</b>	2.93087
<b>Number of Operators</b>	14.0000

Cost of Operating Labor	\$805,000
-------------------------	-----------

As seen in Table 9, the largest impact on the NPV came from major changes in the following: revenue, raw materials, utilities, and labor. After being able to eliminate the bottom recycle stream and other pieces of equipment, we were able to produce \$2 million/year more of fuel gas. Since one of the constraints of the project was a specific production rate of ethylbenzene, the revenue could only be changed by increasing sales of fuel gas. This increase in fuel gas increased the revenue from \$112.9 million in the base

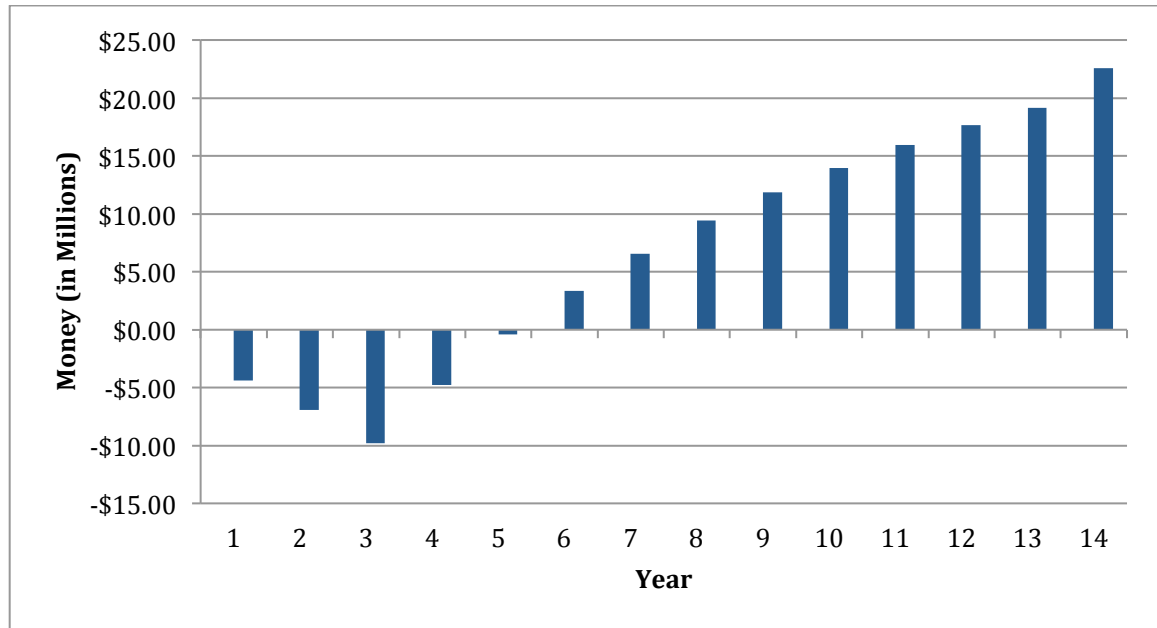


case to \$115 million in the final optimized case. As previously explained by Figure 2, the change in raw materials had the greatest impact on the project's worth. In the optimized case, the raw materials cost decreased by \$9 million, yielding a revised cost of \$76.6 million.

The utilities cost for the optimized case, which ended up at \$120,000/year, was another factor of the increased net present value, as it presented a significant decrease from the base case utilities cost, \$924,600/year. The bulk of the utilities cost came from the fired heater, which had to heat the stream up to 370°C before the stream entered the reactor chain. By eliminating the bottom recycle stream, we were able to eliminate the need for that stream to be heated by the fired heater. This was decreased the required duty of the heat exchanger from 25,500 MJ/hour to 19,400 MJ/hour, thus decreasing the fired heater's utility cost from \$2.35 million/year to \$1.8 million/year. Additionally, the removal of three pumps, one on the eliminated distillation column and the other two eliminated from the unnecessary recycle streams, decreased the utility cost. Finally, the removal of four heat exchangers, two on T-302 and two eliminated before two of the reactors in the reactor chain, further decreased the utility cost. The largest impact on the utility cost arose from the decreased duty of the fired heater.

Labor cost, directly related to the amount of nonparticulate processing steps, also saw a decrease. In the base case, which included 16 of these processing steps, the labor cost totaled \$862,500/year. By eliminating a distillation column, four heat exchangers, and one reactor, the number of processing steps dropped from 16 to 10. This dropped the number of operators to 2.9/shift and lead to a lowered cost of \$805,000/year.

Overall, the changes made during the optimization process improved our project from -\$11.1 million to \$22.5 million. It also gave us a conventional payback period, or the time required for the project to break even, at a value of 5.1 years



**Figure 9.** Cumulative cash flow diagram, optimized case.

In conclusion, we would state that these optimizations enhanced and made this project worth an investment.

## **Conclusion and Recommendations:**

In conclusion, we would state that these optimizations made to the original base case enhanced and made this project worth an investment. Going from -\$11.1 million to \$22.5 million is a drastic change in net present value and is directly related to the changes made in the optimization process. Similarly, a payback period of 5.1 years resulted from the optimized case; there was no payback period in the project life of the base case.

When given the option of considering Change 1 (new catalyst), Change 2 (cheaper feed cost, lower grade benzene feed), both changes, or no changes, our group chose both changes due to the increased net present value. When moving on with further optimization from both changes, we decided that a vital part of the optimization would include the elimination of the bottom recycle stream and the improvement of the reactor chain section of the plant. By analyzing the temperature effect on single-pass conversion and selectivity of ethylbenzene in the reactors, we decided that an increased temperature throughout the reactor chain section would allow for the greatest conversion and decrease the amount of feed required. Furthermore, since the reactions taking place were exothermic, the first reactor would increase the temperature for the stream entering the second reactor, and further increase the conversion in each successive reactor. Although this action would require an increase in equipment cost, by using stainless steel materials for the second and third reactors, we deemed it a necessary call to get the highest conversion.

As a direct effect of the higher conversion occurring in the reactors, there was less diethylbenzene being produced and hence no need for a second distillation column separating and recycling the diethylbenzene to a another reactor. By eliminating the bottom recycle stream, we were able to eliminate equipment costs for a distillation tower, reactor, and pump, but what greatly benefitted the net present value was the elimination of the use of the fired heater for the bottom stream. The utility cost per year was decreased from \$900k to \$100k, basically all due to the decreased fired heater duty.

After completion of our optimization, we would recommend further investigation of the feed cost to raise the net present value even more. Judging from the sensitivity

analysis, the raw materials cost is the most efficient way to impact on the net present value. There is a significant amount of benzene escaping in the fuel gas stream; if this can be restored in the recycle stream, less fresh feed will be required, yielding a lower cost of materials. Also, by adding more reactors or changing reactor parameters, such as pressure drop, temperature, and length, we believe that the raw materials feed can be reduced, if the single-pass conversion of each reactor can be further increased. Due to time constraints, we were unable to deeply analyze these changes and how they affected the overall process.

## **Nomenclature**

T-30X – refers to towers and the X refers to the location of the tower in the system

E-30X – refers to heat exchangers and X refers to the location of the heat exchanger in the system

H-30X – refers to fired heater and X refers to the location of the fired heater in the system

P-30X A/B – refers to pumps and X refers to the location of the pump in the system. The A/B means there is a back-up pump

R-30X – refers to reactors and X refers to the location of the reactor in the system

V-30X – refers to vessels and X refers to the location of the reactor in the system

PFD – Process Flow Diagram

SRK – Soave-Redlich-Kwong thermodynamic package

PR – Peng-Robinson thermodynamic package

SRKS – Soave-Redlich-Kwong SIMSCI thermodynamic package

Q – heat in MJ/hr

U – heat transfer coefficient in  $W/m^2/^\circ C$

A – heat transfer area in  $m^2$

$F_t$  – correction factor

$\Delta T_{LM}$  – log mean temperature difference in  $^{\circ}C$

m – mass flow rate in kg/hr

$\Delta H$  – enthalpy in kJ/kg

R – Reflux ratio;  $R_{min}$  is the minimum reflux ratio

N – refers to the number of trays in a tower;  $N_{min}$  is the minimum number of trays while

$N_{actual}$  is the actual number of trays required for the tower.

H – height of the tower in m

$\rho_i$  – density of a substance in  $kg/m^3$

$V_i$  – volumetric flow rate of a stream in  $m^3/hr$

$v_i$  – velocity of a stream in m/s

$d_i$  – diameter of a tower, either top or bottom of tower, in m

BMC – bare module cost

NOL – number of operators

$N_{np}$  – number of nonparticulate processing steps

P – number of processing steps involving the handling of particulate solids

cw – cooling water utility

hps – high pressure steam utility

lps – low pressure steam utility

bfw – boiler feed water utility

MACRS – Modified Accelerated Cost Recovery System

FCI – Fixed Capital Investment

NPV – Net Present Value

## **Safety Aspect**

Chemical plants are well known for their accidents especially those that are tragic. The safety aspect of the plant plays a crucial role to ensure the number of accidents is minimized. Following are some options can be implemented when it comes to safety.

The first safety aspect that we looked into was prevention. Prevention can be done by using safe design methods. Two things that we noticed were the high temperatures and high pressures. Our highest temperature is 495°C and the highest pressure is at 2000kPa. We suggest that insulations be used on the hot pipes to overcome the high temperature and a pressure relief system be used to

- Keep controls and computer software user friendly
- Have well defined instruction and procedures
- Reduce the quantities of materials in the process
- Minimize piping by having a good plant layout
- Use independent sensors for alarmed variables such as the reactants in the reactor.
- Have a good control system especially for emergency shut downs
- Have a good relief system to avoid over pressurization of the reactors and vessels.

# Appendix

# Contents

Sample Calculations .....	46
Pump.....	46
Tower.....	46
Vessel .....	48
Heat Exchanger .....	51
Reactor.....	57
Catalyst Cost.....	57
Cash Flow Statement.....	58
Base Case.....	58
Proposed Change 1 – Change of Catalyst Only .....	59
Proposed Change 2 – Change of Feed Ratio Only .....	60
Proposed Change 1 and 2 – Change of Catalyst and Feed Ratio .....	61
Optimized Case .....	62
Thermodynamic Package Guideline.....	63



## Sample Calculations

### Pump

Heuristics for the pump are obtained from Table 11.9, page 346 of Analysis, Synthesis and Design of Chemical Processes, 4<sup>th</sup> Edition

Heuristic used:

1) Power for pumping liquids;  $kW = (1.67)[\text{Flow}(m^3/\text{min})][\Delta P(\text{bar})]/\eta$

$$W = \frac{1.67 \times \dot{V} \times \Delta P}{\eta}$$

$$W(kW) = \frac{1.67 \times 0.345683 \frac{m^3}{min} \times 18.9 \text{ bar}}{0.75} = 14.5 \text{ kW}$$

### Tower

Heuristics for towers are obtained from Table 11.13 & 11.14 page 350 & 351 of Analysis, Synthesis and Design of Chemical Processes, 4<sup>th</sup> Edition

Heuristic used:

- 1) Economical optimum reflux ratio is in the range of 1.2 to 1.5 times the minimum reflux ratio
- 2) The economically optimum number of theoretical trays is near twice the minimum value of  $N_{\min}$
- 3) A safety factor of 10% of the number of trays calculated by the best means is advisable
- 4) Tray efficiencies for distillation of light hydrocarbons and aqueous solutions are 60-90%

$N_{\min}$  was obtained from the PRO/II simulation.

$$R = (1.2 \rightarrow 1.5) \times R_{min}$$

$$R = (1.2 \rightarrow 1.5) \times 0.41593 = 0.499116 \rightarrow 0.623895$$

$$N_{actual} = \frac{1.1 \times 2 \times N_{min}}{\eta}$$

$$N_{actual} = \frac{1.1 \times 2 \times 7.63}{0.75} = 22.38 = 23 \text{ Trays}$$

$$H = 0.5 \times N_{actual} + 3$$

$$H = 0.5 \times 23 + 3 = 14.5$$

$m$

$$\rho_i = \frac{\dot{m}_i}{\dot{V}_i}$$

$$\rho_i = \frac{13578.34 \frac{kg}{hr}}{3926.19 \frac{m^3}{hr}} = 3.458 \frac{kg}{m^3}$$

$$v_i = \frac{(1.2 \rightarrow 1.5) \frac{m}{s} \times \frac{kg^{0.5}}{m^3}}{\rho_i^{0.5}}$$

$$v_i = \frac{1.2 \rightarrow 1.5 \frac{m}{s} \times \left(\frac{kg}{m^3}\right)^{0.5}}{\left(3.458 \frac{kg}{m^3}\right)^{0.5}} = (0.645 \rightarrow 0.807) \frac{m}{s}$$

$$d_i = \frac{4 \times \dot{V}_i^{0.5}}{\pi \times v_i}$$

$$d_i = \frac{4 \times 3926.19 \frac{kg}{hr}^{0.5}}{\pi (0.645 \rightarrow 0.807) \frac{m}{s}} = (1.47 \rightarrow 1.31) m$$

## Vessel

The heuristics used can be found on Table 11.6, page 344 of Analysis, Synthesis and Design of Chemical Processes, 4<sup>th</sup> Edition

### V-301 (base-case)

Heuristic used:

- 1) In drums feeding a furnace, 30 min for a half full drum is allowed.
- 2) Optimum ratio of length to diameter =3, but the range 2.5 – 5 is common

Flow rate out (from PRO/II): 20.725 m<sup>3</sup>/hr

Holdup Time: 30 minutes

$$Volume = (Flowrate \times Holdup Time) \times 2$$

$$Volume = \left( 20.725 \frac{m^3}{hr} \times 30 \text{ mins} \right) \times 2 = 20.725 m^3$$

$$Volume = \pi \times \frac{D^2}{4} \times L$$

$$\frac{L}{D} = 3$$

$$D = \left( \frac{V \times 4}{\pi \times 3} \right)^{\frac{1}{3}}$$

$$D = \left( \frac{20.725 \frac{m^3}{hr} \times 4}{\pi \times 3} \right)^{\frac{1}{3}} = 2.06 \text{ m}$$

$$L = 3 \times D$$

$$L = 3 \times 2.06 \text{ m} = 6.2 \text{ m}$$

### V-302 (base-case)

Heuristic used:

- 1) Holdup time is 5 min for half-full reflux drums and gas/liquid separators
- 2) Optimum ratio of length to diameter = 3, but the range 2.5 – 5 is common

Flow rate out (from PRO/II): 29.4 m<sup>3</sup>/hr

Holdup Time: 5 minutes

$$Volume = (Flowrate \times Holdup Time) \times 2$$

$$Volume = \left( 29.4 \frac{m^3}{hr} \times 5 \text{ mins} \right) \times 2 = 4.9 m^3$$

$$Volume = \pi \times \frac{D^2}{4} \times L$$

$$\frac{L}{D} = 3$$

$$D = \left( \frac{V \times 4}{\pi \times 3} \right)^{\frac{1}{3}}$$

$$D = \left( \frac{4.9 \frac{m^3}{hr} \times 4}{\pi \times 3} \right)^{\frac{1}{3}} = 1.27 \text{ m}$$

$$L = 3 \times D$$

$$L = 3 \times 1.27 \text{ m} = 3.8 \text{ m}$$

### V-303 (base-case)

Heuristic used:

1) Holdup time is 5-10 min for a product feeding another tower

2) Optimum ratio of length to diameter =3, but the range 2.5 – 5 is common

Due to the reflux pumped back to the tower, calculation of this vessel differs.

Returned: 97.9 kmol/hr

Density: 875.25 kg/m<sup>3</sup>

Product: 174.9 kmol/hr

Holdup Time: 10 minutes

MW: 77.52 kg/kmol

$$\text{Flowrate} = \frac{(\text{Returned} + \text{Product}) \times \text{MW}}{\rho}$$

$$\text{Flowrate} = \frac{\left(97.9 \frac{\text{kmol}}{\text{hr}} + 174.9 \frac{\text{kmol}}{\text{hr}}\right) \times 77.52 \frac{\text{kg}}{\text{kmol}}}{875.25 \frac{\text{kg}}{\text{m}^3}} = 24.2 \frac{\text{m}^3}{\text{hr}}$$

$$\text{Volume} = (\text{Flowrate} \times \text{Holdup Time}) \times 2$$

$$\text{Volume} = \left(24.2 \frac{\text{m}^3}{\text{hr}} \times 10 \text{ mins}\right) \times 2 = 8.05 \text{ m}^3$$

$$\text{Volume} = \pi \times \frac{D^2}{4} \times L$$

$$\frac{L}{D} = 3$$

$$D = \left( \frac{V \times 4}{\pi} \right)^{\frac{1}{3}}$$

$$D = \left( \frac{8.05 \frac{m^3}{hr} \times 4}{\pi} \right)^{\frac{1}{3}} = 1.5 m$$

$$L = 3 \times D$$

$$L = 3 \times 1.5 m = 4.5 m$$

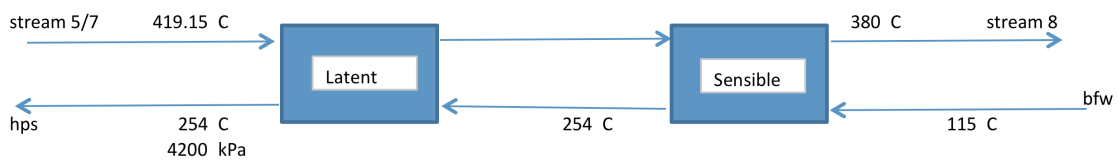
## Heat Exchanger

The heuristics used were obtained from table 11.11 page 348 of Analysis, Synthesis and Design of Chemical Processes, 4<sup>th</sup> Edition

**E-301 (base-case)**, [calculation is repeated for E-302 to E-304]

Heuristic used:

- 1) Heat transfer coefficient for estimating purposes for liquid to gas is  $60 \text{ W/m}^2\text{C}$



From steam tables found in Elementary Principles of Chemical Processes, R.Felder and R.Rousseau, Appendix B, Table B6 from pages 644-649 & Table B7 from pages 650-651:

H at 254 C, 4200 kPa, hps = 2800 kJ/kg

H at 254 C, liq = 1101 kJ/kg

H at 115 C, liq, bfw = 485.4 kJ/kg

Q from Pro/II = 1824 MJ/h

$$Q = m \times \Delta H$$

$$m = \frac{1824 \frac{MJ}{hr}}{(2800 - 1101) \frac{kJ}{kg}} = 788 \frac{kg}{hr}$$

$$Q_{sensible} = (1101 - 485.4) \frac{kJ}{kg} \times 788 \frac{kg}{hr} = 485.1 \frac{MJ}{hr}$$

$$Q_{latent} = (2800 - 1101) \frac{kJ}{kg} \times 788 \frac{kg}{hr} = 1338.9 \frac{MJ}{hr}$$

$$\frac{Q_{Latent}}{Q_{Total}} = \frac{C_p(T_{Latent} - T)}{C_p(T_{Latent} - T_{Sensible})}$$

$$\frac{1338.9 \frac{MJ}{hr}}{1824 \frac{MJ}{hr}} = \frac{C_p(419.15 - T)}{C_p(419.15 - 380)}$$

$$T = 390.4^\circ\text{C}$$

$$\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{\ln \frac{\Delta T_1}{\Delta T_2}}$$

For sensible side ( $F_T=0.9$ ):

$$\Delta T_1 = (390.4 - 254)^\circ\text{C} = 136.4^\circ\text{C}$$

$$\Delta T_2 = (380 - 115)^\circ\text{C} = 265^\circ\text{C}$$

$$\Delta T_{LM} = \frac{136.4^\circ\text{C} - 265^\circ\text{C}}{\ln \frac{136.4^\circ\text{C}}{265^\circ\text{C}}} = 193.6^\circ\text{C}$$

$$Q = UAF_T\Delta T_{LM}$$

$$A_{Sensible} = \frac{485.1 \frac{MJ}{hr}}{60 \frac{W}{(m^2 \cdot ^\circ C)} \times 0.9 \times 193.6^\circ C} = 12.9 m^2$$

For latent side ( $F_T=1$ ):

$$\Delta T_1 = (390.4 - 254)^\circ C = 136.4^\circ C$$

$$\Delta T_2 = (419.15 - 254)^\circ C = 165.19^\circ C$$

$$\Delta T_{LM} = \frac{136.4^\circ C - 165.19^\circ C}{\ln \frac{136.4^\circ C}{165.19^\circ C}} = 150.3^\circ C$$

$$Q = UAF_T\Delta T_{LM}$$

$$A_{Latent} = \frac{1338.9 \frac{MJ}{hr}}{60 \frac{W}{(m^2 \cdot ^\circ C)} \times 1 \times 150.3^\circ C} = 41.2 m^2$$

$$Total Area = A_{Sensible} + A_{Latent}$$

$$Total Area = 12.9 m^2 + 41.2 m^2 = 54.1 m^2$$

### E-306 (base-case) [tower reboiler]

Heuristic used:

- 1) Heat transfer coefficient for estimating purposes for reboiler is  $1140 \text{ W/m}^2\text{C}$
- 2) Maximum flux in reboiler is  $31.5 \text{ kW/m}^2$





$F_T=1$

Q from Pro/II = 10866 MJ/h

$$Q = UAF_T\Delta T_{LM}$$

$$\Delta T_{LM} = T_2 - T_1$$

$$\Delta T_{LM} = 160 - 146 = 14^\circ\text{C}$$

$$A = \frac{10866 \frac{\text{MJ}}{\text{hr}}}{1140 \frac{\text{W}}{(\text{m}^2\text{C})} \times 1 \times 14^\circ\text{C}} = 189.4 \text{ m}^2$$

$$q = \frac{Q}{A}$$

$$q = \frac{10866 \frac{\text{MJ}}{\text{hr}}}{189.4 \text{ m}^2} = 15.9 \frac{\text{kW}}{\text{m}^2}$$

Since  $q$  obtained is less than  $q_{\text{max}}$ . This area is valid.

### E-308 (base-case) [tower reboiler]



Heuristics used:

- 1) Heat transfer coefficient for estimating purposes for reboiler is  $1140 \text{ W/m}^2\text{C}$
- 2) Maximum flux in reboiler is  $31.5 \text{ kW/m}^2$

$F_T=1$

Q from Pro/II = 6098 MJ/h

$$Q = UAF_T\Delta T_{LM}$$

$$\Delta T_{LM} = T_2 - T_1$$

$$\Delta T_{LM} = 254 - 149.8 = 104.2^\circ\text{C}$$

$$A = \frac{6098 \frac{\text{MJ}}{\text{hr}}}{1140 \frac{\text{W}}{(\text{m}^2\text{C})} \times 1 \times 104.2^\circ\text{C}} = 14.2 \text{ m}^2$$

$$q = \frac{Q}{A}$$

$$q = \frac{6098 \frac{\text{MJ}}{\text{hr}}}{14.2 \text{ m}^2} = 118.8 \frac{\text{kW}}{\text{m}^2}$$

Since q is greater than  $q_{\max}$ . We used  $q_{\max}$  of  $31.5 \text{ kW/m}^2$  to find area.

$$A = \frac{Q}{q_{\max}}$$

$$A = \frac{6098 \frac{\text{MJ}}{\text{hr}}}{31.5 \frac{\text{kW}}{\text{m}^2}} = 53.8 \text{ m}^2$$

### E-307 (base-case) [tower condenser]



Heuristics:

- 1) Heat transfer coefficient for estimating purposes for condenser is  $850 \text{ W/m}^2\text{C}$

$F_T=1$

Q from Pro/II = 9657 MJ/h

$$Q = UAF_T\Delta T_{LM}$$

$$\Delta T_{LM} = T_2 - T_1$$

$$\Delta T_{LM} = 50.77 - 30 = 20.77^\circ\text{C}$$

$$A = \frac{9657 \frac{\text{MJ}}{\text{hr}}}{850 \frac{\text{W}}{(\text{m}^2\text{C})} \times 1 \times 20.77^\circ\text{C}} = 152 \text{ m}^2$$

## Reactor

### Individual Reactor Volume

$$V_i = \pi * \frac{D_i^2}{4} * L_i$$

$$V_1 = \pi * \frac{(1.72m)^2}{4} * 8.62m = 20.0m^3$$

Total volume of the reactors:

$$\text{Total Volume of Reactors} = (20 + 25 + 30 + 1.67)m^3 = 76.67m^3$$

## Catalyst Cost

*Cost of Catalyst*

$$= (\text{Total Volume of Reactors}) * \rho_i * (\text{void fraction}) \\ * (\text{cost per kg})$$

$$\text{Cost of Base Catalyst} = 76.67m^3 * 1200 \frac{kg}{m^3} * 0.4 * \frac{\$5}{kg} = \$460,020 \text{ every 3 years}$$

$$\text{Cost of New Catalyst} = 76.67m^3 * 1250 \frac{kg}{m^3} * 0.4 * \frac{\$8}{kg} = \$306,680 \text{ every 4 years}$$

# Cash Flow Statement

## Base Case

Income Statement	1	2	3	4	5	6	7	8	9	10	11	12	13	14
End of Year														
Revenue			112929407	112929407	112929407	112929407	112929407	112929407	112929407	112929407	112929407	112929407	112929407	112929407
Expenses														
Materials			86020499.3	85560479.3	86020499.3	85560479.3	85560479.3	86020499.3	85560479.3	85560479.3	86020499.3	85560479.3	85560479.3	85560479.3
Labor			862500	888375	915026.25	942477.038	970751.349	999873.889	1029870.11	1060766.21	1092589.2	1125366.87	1159127.88	1193901.71
Utilities			924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216	924635.216
Others			22635807.5	22574766.6	22620873.3	22774167.8	22717277.7	22767659.7	22925357.8	22873003.4	22928057.2	23090567.2	23043169.1	23103327.9
Depreciation														
Building/Machines			1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05
Taxable Income			1259729.81	1754915.66	1682157.75	1041392.5	1530028.23	1450523.69	802809.423	1284287.66	2423645.96	1768338.3	2241995.35	2147062.78
Income Taxes			568878.415	789712.048	756970.987	468626.625	688512.704	652735.663	361264.24	577929.448	1090640.68	795752.235	1008897.91	966178.251
Net Income			692851.397	965203.614	925186.762	572765.875	841515.527	797788.032	441545.183	706358.214	1333005.28	972586.065	1233097.44	1180884.53
<b>Cash Flow Statement</b>														
Operating Activities														
Net Income			692851.397	965203.614	925186.762	572765.875	841515.527	797788.032	441545.183	706358.214	1333005.28	972586.065	1233097.44	1180884.53
Depreciation			1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05	1226235.05
Investment Activities														
Land														
Buildings/Machines			-5148642.6	-3432428.4										858107.1
Gains Tax														
Land														
Buildings/Machines														
Working Capital			-14552375	-70201.25	-63538.438	19994.2594	-49607.163	-42326.528	41842.5264	-27103.448	-19147.701	65716.7178	-2513.0307	14447662
Net Cash Flow			-5148642.6	-3432428.4	-13859523	895002.364	861648.325	592760.134	791908.364	755461.504	483387.709	679254.766	1313857.57	1038302.78
Cumulative Cash Flow			-5148642.6	-8581071	-22440594	-21545592	-20683944	-20091184	-19299275	-18543814	-18060426	-17381171	-16067314	-15029011
Present Value			-4477080.5	-2595409	-9112861.7	511720.506	428391.501	256266.564	297707.686	246961.706	137408.956	167901.39	282404.781	194066.214
Cumul Discounted CF			-4477080.5	-7072489.5	-16185351	-15673631	-15245239	-14988973	-14691265	-14444303	-14306894	-14138993	-13856588	-13662522
Net Present Value			-11132481											
NPV			\$ (11,132,480.88)											

**Proposed Change 1 – Change of Catalyst Only**

<b>Income Statement</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>	<b>11</b>	<b>12</b>	<b>13</b>	<b>14</b>	
End of Year															
Revenue			112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991	112873991
Expenses															
Materials		86455691.1	86149011.1	86149011.1	86149011.1	86149011.1	86455691.1	86149011.1	86149011.1	86149011.1	86455691.1	86149011.1	86149011.1	86149011.1	86149011.1
Labor		862500	888375	915026.25	942477.038	970751.349	999873.889	1029870.11	1060766.21	1060766.21	1092589.2	1125366.87	1159127.88	1193901.71	1193901.71
Utilities		795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764	795274.764
Others		22690409.9	22664637.2	22710743.9	22758233.7	22877684.7	22857530.3	22909423.8	22962874	23088464.2	23074633.2	23133039.7	23193198.4	23193198.4	23193198.4
Depreciation															
Building/Machines			1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71
Taxable Income		860716.855	1167294.5	1094536.59	1019595.94	565190.673	862902.538	781012.866	696666.504	1441972.06	1729705.41	1637537.86	1542605.29	1542605.29	1542605.29
Income Taxes		387322.585	525282.527	492541.467	458818.174	254335.803	388306.142	351455.79	313499.927	648887.428	778367.433	736892.037	694172.379	694172.379	694172.379
Net Income		473394.27	642011.978	601995.126	560777.768	310854.87	474596.396	429557.076	383166.577	793084.634	951337.974	900645.823	848432.908	848432.908	848432.908
<b>Cash Flow Statement</b>															
Operating Activities															
Net Income		473394.27	642011.978	601995.126	560777.768	310854.87	474596.396	429557.076	383166.577	793084.634	951337.974	900645.823	848432.908	848432.908	848432.908
Depreciation		1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71	1209398.71
Investment Activities															
Land															
Buildings/Machines		-5077951.2	-3385300.8												846325.2
Gains Tax															
Land															
Buildings/Machines															
Working Capital		-14624907	-44644.583	-37981.771	-31119.074	27062.8372	-16769.861	-9270.8069	-1546.7811	57522.2988	14603.3844	23043.636	14447662	14447662	14447662
Net Cash Flow		-5077951.2	-3385300.8	-1415151.3	597367.394	564013.355	529658.694	337917.707	457826.535	420286.269	381619.796	850606.933	965941.359	923689.459	16142420.1
Cumulative Cash Flow		-5077951.2	-8463252	-22614765	-22017397	-21453384	-20923725	-20585807	-20127981	-19707695	-19326075	-18475468	-17509527	-16585837	-443416.97
Present Value		-4415609.7	-2559773.8	-9304849.2	341546.746	280414.318	228986.07	127035.783	149664.306	119471.589	94330.5772	182832.196	180541.347	150125.36	2281386.57
Cumul Discounted CF		-4415609.7	-6975383.5	-16280233	-15938686	-15658272	-15429286	-15302250	-15152586	-15033114	-14938783	-14755951	-14575410	-14425284	-12143898
Net Present Value		-12143898													
NPV															\$ (12,143,897.88)

## Proposed Change 2 – Change of Feed Ratio Only

Income Statement	1	2	3	4	5	6	7	8	9	10	11	12	13	14
End of Year														
Revenue		116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179	116548179
Expenses														
Materials		79589257.7	79129237.7	79129237.7	79589257.7	79589257.7	79129237.7	79129237.7	79589257.7	79129237.7	79589257.7	79129237.7	79129237.7	79129237.7
Labor		862500	888375	888375	915026.25	942477.038	970751.349	999873.889	1029870.11	1060766.21	1092589.2	1125366.87	1159127.88	1193901.71
Utilities		1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28	1098854.28
Others		21252128.7	21191087.9	21237194.5	21390489	21333598.9	21388980.9	21541679	21489324.7	21544378.4	217068884	21659490.3	21719649.1	
Depreciation														
Building/Machines		1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12
Taxable Income		12459900.8	12955086.7	12882328.8	12241563.5	12730199.2	12650694.7	12002980.4	12484458.7	13683119	13027811.4	13501468.4	13406535.9	
Income Taxes		5606955.37	5829789	5797047.94	5508703.58	5728589.66	5692812.62	5401341.2	5618006.4	6157403.57	5862515.12	6075660.8	6032941.14	
Net Income		6852945.45	7125297.67	7085280.82	6732859.93	7001609.58	6957882.09	6601639.24	6866452.27	7525715.47	7165296.26	7425807.64	7373594.72	
<b>Cash Flow Statement</b>														
Operating Activities														
Net Income		6852945.45	7125297.67	7085280.82	6732859.93	7001609.58	6957882.09	6601639.24	6866452.27	7525715.47	7165296.26	7425807.64	7373594.72	
Depreciation		1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	1285537.12	0
Investment Activities														
Land														
Buildings/Machines		-5397636.6	-3598424.4											899606.1
Gains Tax														
Land														
Buildings/Machines														
Working Capital		-13480501	-7020125	-63538.438	19994.2594	-49607.163	-42326.528	41842.5264	-27103.448	-19147.701	65716.7178	-2513.0307	14447662	
Net Cash Flow		-5397636.6	-3598424.4	-6627555.8	7055096.42	7021742.38	6752854.19	6952002.42	6915555.56	6643481.77	6839348.82	7506567.77	7231012.98	7423294.61
Cumulative Cash Flow		-5397636.6	-8996061	-15623617	-8568520.4	-1546778	5206076.17	12158078.6	19073634.1	25717115.9	32556464.7	40063032.5	47294045.5	54717340.1
Present Value		-4693597	-2720925.8	-4357725.5	4033774.28	3491046.95	2919445.22	2613515.21	2260707.38	1888492.15	1690582.43	1613485.87	1351528.03	1206492.9
Cumul Discounted CF		-4693597	-7414522.9	-11772248	-7738474.1	-4247427.2	-1327982	1285533.26	3546240.64	543732.79	7125315.22	8738801.08	10090329.1	11296822
Net Present Value		14507931.1												
NPV		\$ 14,507,931.07												

## Proposed Change 1 and 2 – Change of Catalyst and Feed Ratio

Income Statement	1	2	3	4	5	6	7	8	9	10	11	12	13	14
End of Year														
Revenue			116187349	116187349	116187349	116187349	116187349	116187349	116187349	116187349	116187349	116187349	116187349	116187349
Expenses														
Materials			78938595	78631915	78631915	78631915	78938595	78631915	78631915	78631915	78938595	78631915	78631915	78631915
Labor			862500	888375	91502625	942477038	970751349	999873889	102987011	106076621	10925892	112536687	115912788	119390171
Utilities			945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487	945231.487
Others			21031141.2	21005368.6	21051475.3	21098965.1	21218416.1	21198261.7	21250155.1	21303605.4	21429195.6	21415364.5	21473771.1	21533929.8
Depreciation														
Building/Machines			1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85
Taxable Income			13162856.5	13469434.1	13396676.2	13321735.6	12867330.3	13165042.2	13083152.5	12998806.1	13781737.8	14069471.2	13977303.6	13882371.1
Income Taxes			5923285.41	6061245.36	6028504.3	5994781	5790298.63	5924268.97	5887418.62	5849462.76	6201782.02	6331262.03	6289786.63	6247066.97
Net Income			7239571.06	7408188.77	7368171.92	7326954.56	7077031.66	7240773.19	7195733.87	7149343.37	7579955.8	7738209.14	7687516.99	7635304.08
<b>Cash Flow Statement</b>														
Operating Activities														
Net Income			7239571.06	7408188.77	7368171.92	7326954.56	7077031.66	7240773.19	7195733.87	7149343.37	7579955.8	7738209.14	7687516.99	7635304.08
Depreciation			1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85	1247024.85
Investment Activities														
Land														
Buildings/Machines														
Gains Tax														
Land														
Buildings/Machines														
Working Capital			-13372057	-44644.583	-37981.771	-31119.074	27062.8372	-16769.861	-9270.8069	-1546.7811	57522.2988	14603.3844	23043.636	14447662
Net Cash Flow			-5235933.6	-3490622.4	-6132486.4	7363544.19	7330190.15	7295835.49	7104094.5	7224003.33	7186463.06	7147796.59	7637478.1	7752812.53
Cumulative Cash Flow			-5235933.6	-8726556	-14859042	-7495498.2	-165308.1	7130527.39	14234621.9	21458625.2	28645088.3	35792884.9	43430363	51183175.5
Present Value			-4552985.7	-2639412	-4032209.4	4210130.29	3644400.01	3154191.02	2670692.26	2361539.5	2042841.32	1766826	1641624.16	1449056.1
Cumul Discounted CF			-4552985.7	-7192397.8	-11224607	-7014476.8	-3370076.8	-215885.83	2454806.43	4816345.93	6859187.26	8626013.26	10267637.4	11716693.5
Net Present Value			16214162.4											
<b>NPV</b>			<b>\$ 16,214,162.38</b>											



## Optimized Case

Income Statement		1	2	3	4	5	6	7	8	9	10	11	12	13	14
End of Year															
Revenue		115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993	115080993
Expenses															
Materials		76952549.7	76645869.7	76645869.7	76645869.7	76645869.7	76645869.7	76645869.7	76645869.7	76645869.7	76645869.7	76952549.7	76645869.7	76645869.7	76645869.7
Labor		805000	829150	854024.5	879645.235	906034.592	93215.63	961212.099	990048.462	1019749.92	1050342.41	1081852.69	1114308.27	1149361.7	1114308.27
Utilities		120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675	120324.675
Others		20242306.2	20213549.3	20256582.2	20300906	20417096	20393582.8	20442016.7	20491903.6	20613823.5	20596212.2	20650724.9	20706873.1	20706873.1	20706873.1
Depreciation															
Building/Machines		1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39
Taxable Income		15759616.5	16070903.4	16002996	15933051.4	15483792	15786804.2	15710373.8	1563150.6	16374545.6	16668244.5	16582221.4	1649361.7	1649361.7	1649361.7
Income Taxes		7091827.41	7231906.52	7201348.19	7169873.12	6967706.41	7104061.89	7069668.23	7034242.75	7368545.52	7500710.01	7461999.64	7422127.96	7422127.96	7422127.96
Net Income		8667789.06	8838996.85	8801647.79	8763178.26	8516085.62	8682742.31	8640705.61	8597407.81	9006000.08	9167534.46	9120221.79	9071489.73	9071489.73	9071489.73
<b>Cash Flow Statement</b>															
Operating Activities															
Net Income		8667789.06	8838996.85	8801647.79	8763178.26	8516085.62	8682742.31	8640705.61	8597407.81	9006000.08	9167534.46	9120221.79	9071489.73	9071489.73	9071489.73
Depreciation		1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39	1201196.39
Investment Activities															
Land															
Buildings/Machines		-5043511.8	-3362341.2												840585.3
Gains Tax															
Land															
Buildings/Machines															
Working Capital															
		-13026675	-45075.833	-38857.208	-32452.025	25258.648	-19059.426	-12060.309	-4851.2179	53687.4789	10222.2699	18099.838	14447662	14447662	14447662
Net Cash Flow		-5043511.8	-3362341.2	-4358885.9	8793921.02	8762790.58	8730726.23	8541344.26	8663682.88	8628645.3	8592556.59	9059687.55	9177756.73	9138321.62	24359737
Cumulative Cash Flow		-5043511.8	-8405853	-12764739	-3970817.9	4791972.71	13522698.9	22064043.2	3077726.1	39356371.4	47948928	57008615.5	66186372.3	75324693.9	99684430.9
Present Value		-4385662.4	-2542413	-2866038.2	5027952.88	4356655.61	3774533.88	3211007.68	2832173.3	2452799.53	2123948.58	1947318.44	1715388.36	1485232.74	3442728.94
Cumul Discounted CF		-4385662.4	-6928075.4	-9794113.7	-4766160.8	-409505.17	3365028.71	6576036.39	9408209.7	11861009.2	13984957.8	15932276.2	17647664.6	19132897.3	22575626.3
Net Present Value		22575626.3													
NPV		\$	22,575,626.28												

# Thermodynamic Package Guideline

