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A GUIDE TO PROCESS OPTIMIZATION

by
Shannon LeeAnn Kynerd

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

Oxford
May 2015

Approved by

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Reader: Dr. Paul Scovazzo

Abstract

Optimization is improving upon an existing process. Generally, the motivation behind optimization is economical. Companies are always looking for ways to improve their process in order to maximize their profit. There are several key steps and strategies that need to be followed in order to guarantee an optimized process and ultimately the maximum profit.

An analysis of the base case is essential to optimization. If the starting point is not fully known, then the amount of progress is not known. The top-down and bottom-up strategies determine the overall procedure for optimization. Top-down begins with the big picture while bottom-up starts with the more specific details. By using both topological optimization and parametric optimization, the layout and the operations of the equipment will be optimized.

Optimization takes time and effort. An in-depth analysis of all changes needs to be performed in order to determine if it is truly beneficial to the base case. In conclusion, as long as the base case has improved, then optimization has occurred.

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Introduction

Optimization is a part of every industry around the world. Companies constantly look for ways to improve their facility in design and operation. The competitive drive behind companies is the main cause for innovation and improvement. Some engineers spend their whole career optimizing existing plants. Each engineer's optimization is different in the end because there are unlimited ways of determining the optimum scenario. The procedure for optimization is well defined, however it leaves the execution of the optimization process open ended.

This thesis is written as a guide to optimization. Different strategies and techniques will be discussed as well as common terminology. The purpose of this thesis is to educate the reader on how to optimize a chemical process. The last section of the thesis is an example of the optimization around a reactor train.

The main five sections of this paper and in the example are defined as:

1. Background
2. Top-Down and Bottom-Up Strategies
3. Base Case
4. Topological Optimization
5. Parametric Optimization

Background

Optimization is best defined as, “The process of improving an existing situation, device, or system such as a chemical process.”(Turton) There is a specific topic or objective function that is the main goal of optimization. Generally the motivation behind optimization is to improve economics. The example demonstrated later in this paper uses the net present value (NPV) as the objective function. There are several decision variables that determine the value of the objective function. The engineer has complete control over these variables and runs analysis on the different parameters to determine if its optimum or not. “Another strategy to determine decision variables is to consider how the process is controlled. Any variable that must be controlled is a decision variable.”(Turton) Another common name for decision variables is design variables. Examples of these are as obvious as the operating temperature and pressure or can be more obscure as the feed tray location in a distillation column. The identification of these decision variables is imperative in the optimization process. After the decision variables are all accounted for, the prominence of each needs to be determined. The list of priorities will narrow down the scope of the optimization. Each process has certain constraints that also need to be known before the process of optimization starts. These constraints can be the purity of the product stream or the maximum temperature in a reactor. The entire process of optimization focuses solely on improving the objective function by using the decision variables while retaining the constraints.

Top-Down and Bottom-Up Strategies

There are two different strategies that can be used to adequately optimize a process, top-down and bottom-up. Top-down focuses on the general picture first then concentrates on the more specific details of the process. Bottom-up is the opposite. It focuses on the more intimate details then the big picture. Generally, top-down is the approach commonly taken. It is easier to see the big picture and develop ideas of optimization before getting too detailed with the area chosen for improvement. However, whichever strategy is chosen should lead to ultimately the same conclusion. Top-down and bottom-up strategies have two steps of optimization, topological and parametric optimization. Nevertheless, the initial step of optimization is the development of a base case.

Base Case

The development of a base case is the initial step of optimization. “Because the goal of optimization is to *improve* the process, it is essential that one start from a defined process, that is, a base case.”(Turton) A detailed analysis of the base case needs to be completed. These details include a process flow diagram, equipment costs, utility costs, raw materials costs, etc. The economics of the base case are extremely important in determining if any changes made during optimization are economical and feasible. The parameters of optimization begin with the base case. This is when the focus shifts to a certain area of the process. Rarely does optimization include the entirety of a process. However, if the scope selected is too narrow, the results of the optimization will be missed and unaccounted for. After choosing the proper parameters and deciding on the objective function and key decision variables, modifications to the process can begin.

Topological Optimization

Topological optimization determines the arrangement of the facility. Topology covers the direction of flow therefore deals with the arrangement of the process equipment. Generally topological optimization is done before parametric optimization. This is because one change in the arrangement or elimination of process equipment has the potential to drastically change the economics of the facility. Because parametric optimization deals with the operating conditions of the process equipment, it is easier if the equipment has already been decided on before beginning parametric optimization.

Deciding on the topology of a facility is mainly dependent on the process characteristics. Turton has identified four key questions that need to be considered thoroughly before beginning. These four questions illustrate the importance of fully understanding the base case before considering optimization.

1. Can unwanted by-products be eliminated?

Unwanted by-products are generally hard to make economical in a facility. Companies hope to eliminate these unwanted by-products by changing the kinetics of the catalyst or adding a recycle stream. These decisions need to be made early on to minimize the amount of time spent optimizing.

2. Can equipment be eliminated or rearranged?

Eliminating and or rearranging equipment is mainly based on understanding the process and the design of the equipment. For example, a compressor is not designed for a liquid stream. It needs to be moved to a different section of the process or needs to be exchanged for something suitable for a liquid like a pump. This is the step that has the biggest change on the economic value of the facility.

3. Can alternative separation methods or reactor configurations be employed?

Separation of a product from byproducts and unwanted reactants is vital to a process. It ensures the purity of the product to be sold. Different techniques of separation exist but the most heavily used is distillation. At this point in topological optimization, justification of adding an additional distillation column needs to be analyzed. Although distillation columns are expensive, if a more pure product can be sold for a higher profit it has potential to be economical. A different reactor configuration is another important option in optimization. Also the type of reactor needs to be justified. The change in the arrangement or type of reactor might directly influence the amount of product therefore changing the equipment needs and sizes. Analysis around the type of reactor and configuration will help determine the best fit for the process.

4. To what extent can heat integration be improved?

Heat integration is the easiest form of topological optimization. The key to heat integration is looking for wasted heat that can replace a utility stream. If a process stream is being cooled with a log mean temperature greater than 100°F, it needs to be justified. If it is not justified then reconfigure the stream by using it instead of a utility stream somewhere else in the facility. An example of heat integration is recognizing that a process stream being cooled by an air cooler from 500°C to 250°C is a waste of heat. This process stream can cool by heating a different process stream that is currently using steam as its heating source. This immediately eliminates the utility costs associated with the steam and the air cooler.

Topological optimization is not difficult in and of itself. It requires creativity and intuition to be able to rearrange equipment to optimize the economic value of the process.

Parametric Optimization

Parametric optimization involves the operations of the equipment. The temperature, pressure, and purity of products are the main area of parametric optimization. The decision variables are closely followed in this type of optimization. If the decision variable is to reduce the size of the tower, then optimization upstream of the tower needs to be done. Changing the reactor temperature or pressure may influence the amount and concentration of the products. If the amount of by-products is reduced then the size of the tower will also be reduced. Another example of parametric optimization is minimizing the time spent in a reactor. Having the residence time as the decision variable can increase the overall profit of the process because of its influence on the amount of product made per year. Optimization of the reactor length as well as the temperature and pressure of the reactor influences the residence time in the reactor. It is imperative, however, to ensure that quality of the product is not lost as a result in reducing the residence time. While changing the conditions of the reactor might seem to be profitable, utilities in the plant need to be monitored to ensure that this change is not shifting the cost elsewhere.

Simulation software is helpful during optimization to reduce the amount of calculations and time spent after every change. Parametric optimization takes longer to perform than topological. An economic analysis needs to be done after every change for it to be clear if a change is warranted.

Topological and parametric optimizations are rarely done in separate settings. Simultaneous use of them is helpful in determining a optimum process. For instance, changing the reactor settings might enable the elimination of other equipment downstream. Joint use of the topological and parametric optimizations seems daunting at first but proves to be the best use of time.

The point of optimization is to make something better. After using the base case as a starting place and determining an area for improvement, the different strategies of optimization will enable the engineer to improve upon the process. Whether top-down or bottom-up strategy is chosen, the steps for topological and parametric optimization are the same. Optimization takes time and effort but in the end is a rewarding process.

Example of Optimization Around a Reactor Train

The following is an example of the optimization done around the reactor section of an ethylbenzene facility.

Base Case

The fresh feed to the facility is benzene that consists of 10 mol% toluene and ethylene that contains 7 mol% ethane. The steam and the 80,000 tonne/yr of ethylbenzene produced in the process are sent to a styrene plant. The prices of the utilities and raw materials are constant throughout the 12 years of the project. In the base case there are four plug flow reactors with three in series. The ratio of the benzene to the ethylene is held constant at 8:1 into the reactor train in order to minimize catalyst poisoning. The simulation of the base case and the optimized case is done in PRO/II using the thermodynamic model of SRK SIMSCI. Case studies calculated in PRO/II are heavily relied upon for the optimization results in this example.

Background

The objective function for the ethylbenzene facility is to maximize the net present value. The constraints for the product ethylbenzene include the purity of the ethylbenzene, which must be precisely 99.8 mol% in order to meet the criteria of the styrene plant. The amount of the by-product diethylbenzene cannot exceed 2 ppm in the product stream. The decision variables include the catalyst and the conditions under which the reactors are operated. The temperature out of the reactors cannot surpass

500°C because of the catalyst constraints. Before starting the steps of optimization, an analysis of the reactions and kinetics on the following four gas-phase reactions is done.

$C_6H_6 + C_2H_4 \longrightarrow C_6H_5C_2H_5$ (1)
benzene ethylene ethylbenzene

$C_6H_5C_2H_5 + C_2H_4 \longrightarrow C_6H_4(C_2H_5)_2$ (2)
ethylbenzene ethylene diethylbenzene

$C_6H_4(C_2H_5)_2 + C_6H_6 \longrightarrow 2\ C_6H_5C_2H_5$ (3)
diethylbenzene benzene ethylbenzene

$C_6H_5CH_3 + 2\ C_2H_4 \longrightarrow C_6H_5C_2H_5 + C_3H_6$ (4)
toluene ethylene ethylbenzene propylene

The reaction kinetics of the base case catalyst are as follows:

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

Table 1: Reaction Kinetics with Base Case Catalyst

i	***E_I*** *kcal/kmol*	***k_{o,i}***	***a***	***b***	***c***	***d***	***e***
1	22500	1.00×10^{6}	1	0	0	1	0
2	22500	6.00×10^{5}	1	1	0	0	0
3	25000	7.80×10^{6}	0	0	0	1	1
4	20000	3.80×10^{8}	2	0	1	0	0

The units of r_i are $\frac{kmol}{s\,m^3}$ reactor, the units of C_i are $\frac{kmol}{m^3}$ gas, and the units of $k_{o,I}$ vary.

Topological Optimization

The base case design of the reactor train demonstrates the potential for improvement in the kinetics of the catalyst and the layout of the reactors. The fourth reactor that is not in the series serves the purpose of converting the by-product diethylbenzene into ethylbenzene. Reaction 3 is inept for the process because the activation energy of this reaction is significantly higher than it is for the more desired reaction 1. A change in catalyst proves to be economical because the new kinetics of the reactions are superior to the base case kinetics. The activation energy of the undesired reaction 2 increases, which translates to the suppression of the diethylbenzene. The favorable reaction 1 increases in activation energy as well but not exponentially as in reaction 3. The kinetics of the new catalyst are shown in Table 2.

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

Table 2: Reaction Kinetics of the New Catalyst

i	***E_I*** *kcal/kmol*	***k_{o,i}***	***a***	***b***	***c***	***d***	***e***
1	22500	1.50×10^6	1	0	0	1	0
2	22500	6.00×10^3	1	1	0	0	0
3	25000	7.80×10^6	0	0	0	1	1
4	20000	3.80×10^8	2	0	1	0	0

The units of r_i are $\frac{kmol}{s\,m^3}$reactor, the units of C_i are $\frac{kmol}{m^3}$ gas, and the units of $k_{o,I}$ vary.

Because of the suppression of the diethylbenzene, topological optimization is fairly simple. The fourth reactor is eliminated immediately since less than 2 ppm diethylbenzene is produced in the reactor train. After changing the catalyst and removing the fourth reactor, parametric optimization is performed on the reactor train.

Parametric Optimization

Various case studies in PRO/II demonstrate the effect of changing the reactor temperatures, pressures, and lengths. Since the rate of reaction is a function of concentration, and the reactions occur in the gas phase, increasing the pressure in the reactors results in a higher conversion of reactants. This is shown in Figure 1. The conclusion of the pressure case studies is that the conversion of benzene levels off around 55% beginning at pressures above 2300 kPa. The optimum pressure is consequently chosen as 2300 kPa.

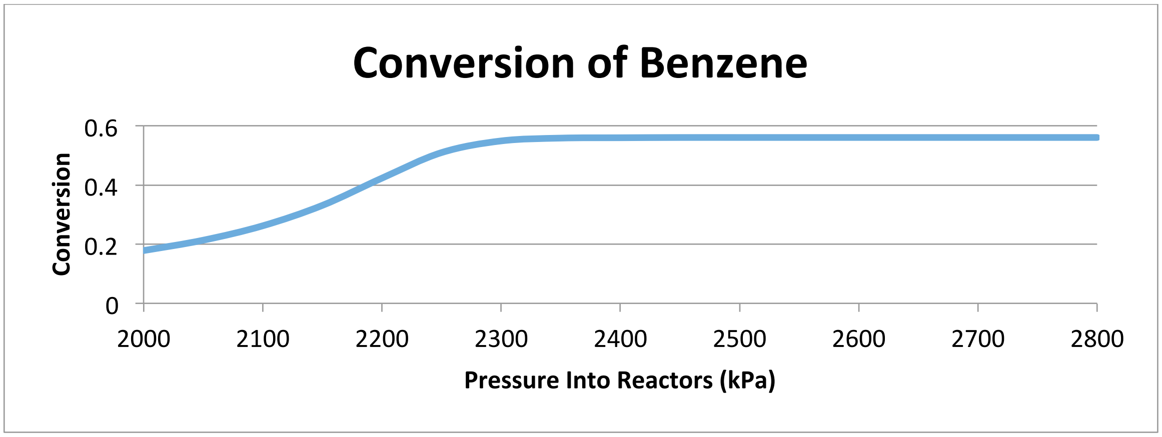

Figure 1: Effect of Reactor Feed Pressure on the Conversion of Benzene

The temperature of the reactors must comply with the constraint of the maximum 500°C exit temperature. The case studies show that the reactions are exothermic and increase in temperature significantly when an adequate amount of ethylene reacts with the benzene. Figure 2 shows that the entry temperature of 280°C into the reactor train is desirable for the production of ethylbenzene. This optimum temperature of 280°C also stays below the maximum 500°C exit temperature.

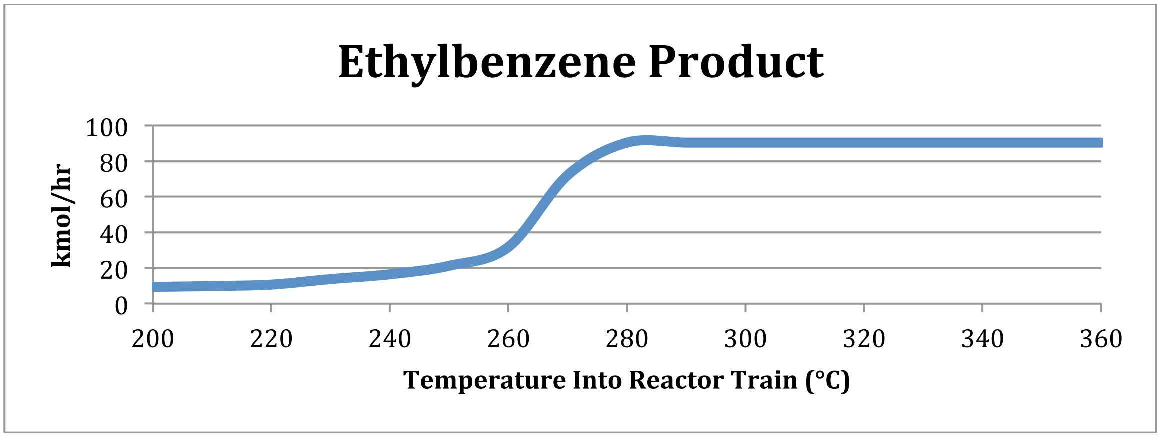

Figure 2: Temperature Into the Reactors Determines the Amount of Products Formed

In determining the total packed bed length that provides an optimal thermal profile, case studies in PRO/II analyze the production of ethylbenzene and the conversion of benzene while ranging in lengths from 1 to 15 meters. Figure 3 shows the results of the case study. 11.9 meters is chosen as the optimum length for the reactors due its high conversion of benzene and it being the smallest available length for the high conversion.

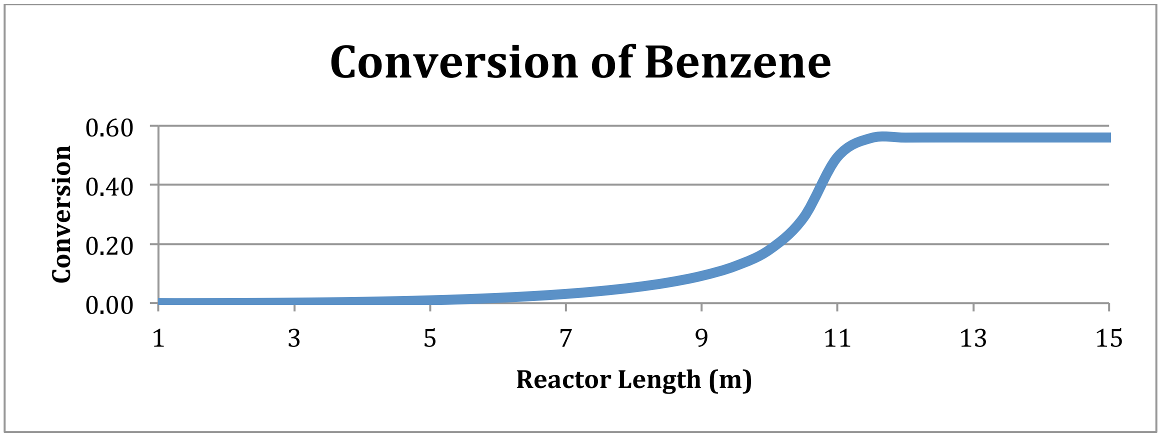

Figure 3: Reactor Length Effect on the Conversion of Benzene

Simultaneous Topological and Parametric Optimization

The results of the parametric optimization of the reactor train offer the opportunity for additional topological optimization. The third reactor in the series is essentially not having any reactions take place because of the temperatures, pressures, and lengths chosen as optimum. Consequently the third reactor is removed. Because of the use of high temperatures and pressures, the materials of choice for the reactors is updated to stainless steel. Optimization is now complete for the reactor train.

Conclusion

Optimization for the reactors in the ethylbenzene facility follows the objective function of improving the net present value of the facility. By using both topological and parametric optimization, the decision variables are chosen as the temperature, pressure, and reactor length. In conclusion, the optimum pressure is chosen as 2300 kPa, temperature as 280°C, and reactor length as 11.9m. All of the constraints are met accordingly and 80,000 tonnes/yr of ethylbenzene product is sent to the styrene plant.

Bibliography

Turton, Richard. *Analysis, Synthesis, and Design of Chemical Processes*. Upper Saddle River, NJ: Prentice Hall, 2012. Print.

Senior Design Project Teammates: Jessica Forbus and Travis Offield

Appendix

Senior Design Project: Ethylbenzene Production Facility

Letter of Transmittal

To: Dr. Smith

From: Jessica Forbus, Shannon Kynerd, and Travis Offield

Date: December 8,2014

Our team optimized the production of an ethylbenzene facility after simulating the base case given in the Senior Design class. Increasing the net present value of the facility was the main objective given. Two initial options of changing the benzene feed to a lower quality and changing to a new catalyst that suppresses the formation of the undesired product, diethylbenzene, significantly helped increase the net present value of the facility.

By using the two main options the net present value increased to $34 million instantly. After further optimization we found that removing multiple pieces of process equipment, including the second distillation tower and the fourth reactor, possible. The final net present value of the facility is $36 million.

Enclosed in our report is a full discussion of our recommendations that the OM Petrochemical facility consider to increase the overall net present value of the facility. We will also provide justifications for our calculations and recommendations.

Jessica Forbus
Shannon Kynerd
Travis Offield

Senior Design 451: Optimization of an Ethylbenzene Production Plant

December 8, 2014

Group 4:
Jessica Forbus
Travis Offield
Shannon Kynerd

Executive Summary

Our team optimized the production of an ethylbenzene plant given a base case. The specifications for the ethylbenzene product are very specific due to the sister styrene plant receiving the entire product of ethylbenzene. The ethylbenzene needs a purity of 99.8% ethylbenzene and less than 2ppm of the byproduct, diethylbenzene. After simulating the base case in PRO II software and discovering the net present value of the base case to be $-10 million, our team chose to investigate several ways to optimize the plant in order to increase the net present value.

The first step in optimization is to perform a sensitivity analysis. This graph determines the variable that has the greatest effect on the value of the net present value. Figure 1 demonstrates that the amount of raw materials and the amount of product, ethylbenzene, have the greatest effect on the net present value. Because the amount of product is fixed at 80,000 tonne/yr due to the styrene plant capacity, our team focuses on the optimization of the raw materials to increase the net present value.

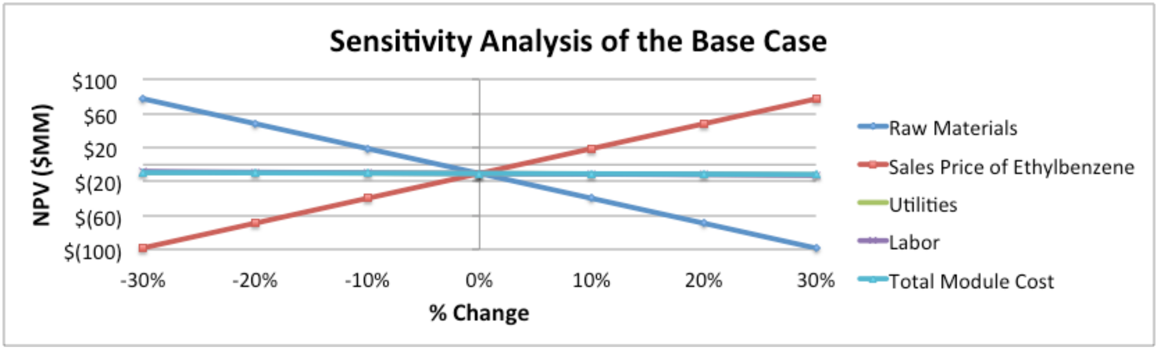

Figure 1: Raw Materials and Price of Ethylbenzene Show the Greatest Effect on the NPV

Our team investigates two options fully to determine their effect on the net present value. The first option involves a change in catalyst from the base case. The new catalyst increases the amount of ethylbenzene out of the reactors by 1.79% and decreases the amount of diethylbenzene in the reactors by 99.48%. The change of the catalyst influences the net present value greatly by increasing it to $4 million.

The second option involves reducing the quality of the benzene from 97% benzene and 3% toluene to a cheaper benzene that consists of 90% benzene and 10% toluene. The effect of only changing the feed proves to be significant. The amount of ethylbenzene produced in the reactors increases by 22.8%. However, the amount of diethylbenzene increases by 142.5% also. The net present value increased to $28 million by using the lower quality benzene feed.

While both options prove profitable by increasing the net present value, utilizing both options was by far the most economical. The amount of ethylbenzene out of the reactors increases by 22.2% and the amount of diethylbenzene in the reactors decreases by 98.5%. The net present value of using both changes proves to be best at $34 million. Therefore; our team fully optimizes the ethylbenzene plant using both the catalyst change and the lower quality benzene.

Our team optimizes the pressure, temperature, and length of the reactor train by using case studies in PRO II. The main source of comparison while changing the pressure, temperature, and reactor length is the conversion of benzene and the amount of diethylbenzene that forms in the reactors. In the case studies, only one variable changes as to see the true effect it has on the products.

The optimum pressure from the case study is 2490 kPa into the reactor train. The higher pressure increases the conversion of the benzene while also lowering the amount of diethylbenzene in the product stream to below 2 ppm. The optimum temperature is 281°C into the reactor train. Although this is lower than expected it is justified because the reactions are extremely exothermic and the outlet temperature in the reactors must be below the maximum temperature of 500°C in order to not hinder the catalyst's life. The optimum length in the reactors proves to be 11.9 m. The trend demonstrates that the larger the length of the reactor, the higher the conversion of the benzene. However, if the length is too large it is no longer economical with the amount of catalyst needed to fill the reactor.

The separator is the last step in the optimization. An optimizer in PRO II determines the optimum pressure and feed tray location by minimizing the duties of the condenser and reboiler. Another factor considered is the amount of benzene lost as fuel gas in the vapor overhead of the column. In order to minimize the amount of benzene in the fuel gas, the pressure changes from 110 kPa to 600 kPa. This increase in pressure reduces the percentage of benzene as fuel gas from 8% of the benzene feed to 1% of the initial benzene feed. Tray 12 in the column gives the optimum outcomes. The column thus gives the best results of low duties on the condenser and reboiler while also keeping the amount of benzene released as fuel gas low.

Our group increases the net present value of the base case from the initial $-10 million to $36 million. Our group recommends utilizing the catalyst change and the lower benzene quality. We also advise to operate the plant at higher pressures and temperatures. Doing this will optimize the plant without compromising the integrity of the product, ethylbenzene.

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Introduction

Our team simulates an ethylbenzene (EB) production plant under given base case conditions, and performs the analysis of a net present value (NPV) to determine the project's economic feasibility. Upon the simulation and evaluation of the base case scenario, our team optimizes the production process by incorporating changes that increase profitability while still adhering to safety protocol and meeting the rigid process specification of producing 80,000 tonne/yr of 99.8 mol% EB containing no more than 2 parts per million (ppm) diethylbenzene (DEB). The optimization process includes, but is not limited to, exploring two possible alternatives from our suppliers: 1) a more expensive, more favorable catalyst, and 2) a cheaper, lower quality benzene feed. Our team investigates the effects of various operating parameters and topological changes as we sought the most efficient method of meeting the production requirements. Ignored from the optimization process was heat integration, as we assume heat integration already exists in a sister styrene plant.

A concept diagram in Figure 2, that outlines the production of EB and fuel gas from benzene and ethylene shows the main sections of the facility to be the reactor and separation section. The economic potential (Table 1) shows the motivation for this project from a business perspective, supplementing our team's motivation to familiarize ourselves with chemical process optimization through this work. We use PRO II software for process simulations and follow chemical process principles and heuristics outlined in Turton's Chapter 11: Utilizing Experience-Based Principles to Confirm the Suitability of a Process Design. We conduct our work under the assumptions that raw material costs, product values, and taxation rates remain constant throughout the 12-year length of the project.

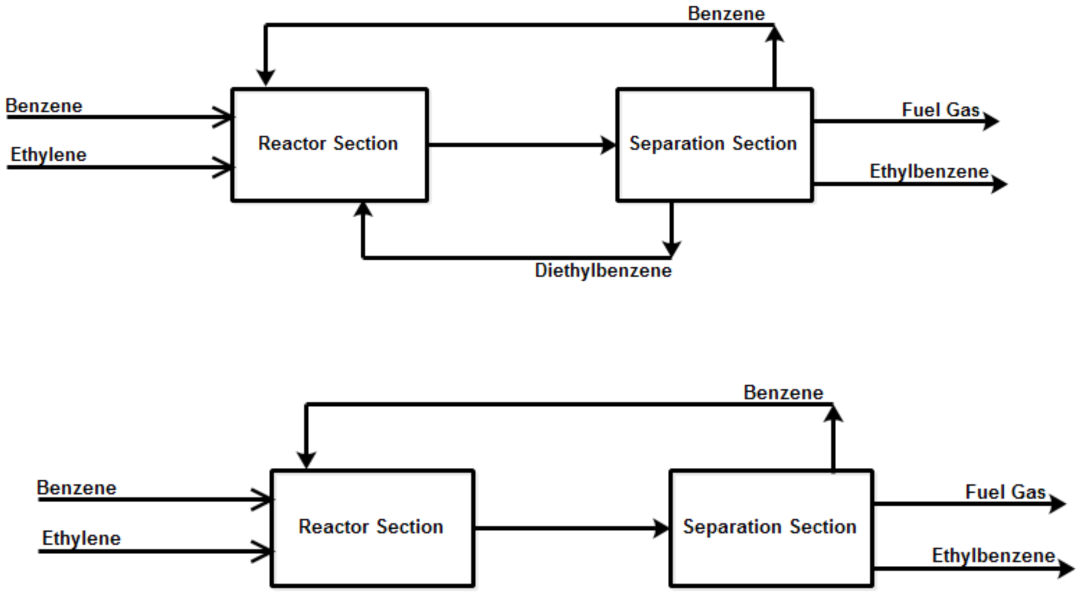


Figure 2: Base Case and Optimized Case Process Diagram

Table 1: Economic Potential of the Ethylbenzene Plant With the Differing Benzene Price

Benzene Price	**Profit Margin**	
$ / kg	$ / kg EB	$MM / year
1.04	0.387	30.9
0.85	0.526	42.1

Results and Discussion

Simulations follow a modified SRK thermodynamic model by using the Thermodynamic Package Diagram. This modified SRK thermodynamic model designs processes that use aromatic hydrocarbons. Further justification of this thermodynamic model follows from the additional use of light hydrocarbons and high operating temperatures (T > 250 K). The following four gas-phase reactions define the production of ethylbenzene, diethylbenzene, and propylene by utilizing the direct addition reaction between the feeds: benzene and ethylene.

C_6H_6 + C_2H_4 ➔ $C_6H_5C_2H_5$ (1)
benzene ethylene ethylbenzene
$C_6H_5C_2H_5$ + C_2H ➔ $C_6H_4(C_2H_5)_2$ (2)
ethylbenzene ethylene diethylbenzene
$C_6H_4(C_2H_5)_2$ + C_6H_6 ➔ 2 $C_6H_5C_2H_5$ (3)
diethylbenzene benzene ethylbenzene
$C_6H_5CH_3$ + 2 C_2H_4 ➔ $C_6H_5C_2H_5$ + C_3H_6 (4)
toluene ethylene ethylbenzene propylene

The reaction kinetics of the base case catalyst is as follows:

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

Table 2: Reaction Kinetics with Base Case Catalyst

i	***E*** E_I *kcal/kmol*	$k_{o,i}$	***a***	***b***	***c***	***d***	***e***
1	22500	1.00×10^6	1	0	0	1	0
2	22500	6.00×10^5	1	1	0	0	0
3	25000	7.80×10^6	0	0	0	1	1
4	20000	3.80×10^8	2	0	1	0	0

The units of r_i are $\frac{kmol}{s\,m^3}$ reactor, the units of C_i are $\frac{kmol}{m^3}$ gas, and the units of $k_{o,I}$ vary.

Base Case Process Description

The ethylbenzene production facility has two feed streams, benzene and ethylene, that when fed into a series of reactors produce ethylbenzene and fuel gas. The benzene feed stream is fed into a surge drum, V-301, along with the recycle benzene from downstream in the plant. The combined benzene is pressurized to 2000 kPa by a positive displacement pump, P-301. This stream then is heated to approximately 400°C by the radiant section of a fired heater, H-301. The heated benzene is mixed with ethylene and enters into a series of adiabatic reactors R-301 to R-303. Ethylene is added between the reactors to replenish what reacted and converted to product. Because the reactions are exothermic, a heat exchanger is placed between the reactors to cool the product to 380°C. These exchangers, E-301 and E-302, use boiler feed water to produce high-pressure steam to be used in the styrene plant. After the third reactor, a series of three exchangers, E-303 to E-305 cools the products to approximately 80°C. Each of these exchangers produces either steam or returns as cooling water.

This newly cooled product stream enters a vessel, V-302, where the vapor is sent out of the plant as fuel gas and the liquid from the vessel is sent to the first distillation column, T-301. The unreacted benzene is condensed out of the top of the tower and sent to the surge drum, V-301, as recycled benzene. The bottoms product enters into a second distillation column, T-302, where the top product, ethylbenzene is sent directly to the styrene plant. The bottom's product out of the column is mainly the undesired byproduct, diethylbenzene. Using the pump, P-304, the diethylbenzene is sent through the convective section of the fired heater, H-301, after mixing with recycled benzene. This heated stream enters into a fourth adiabatic reactor, R-304, where it is reacted to form ethylbenzene. This stream mixes with the reactor products of R-303 into the first cooling exchanger, E-303.

Figure 3: Process Flow Diagram of the Base Case Part 1

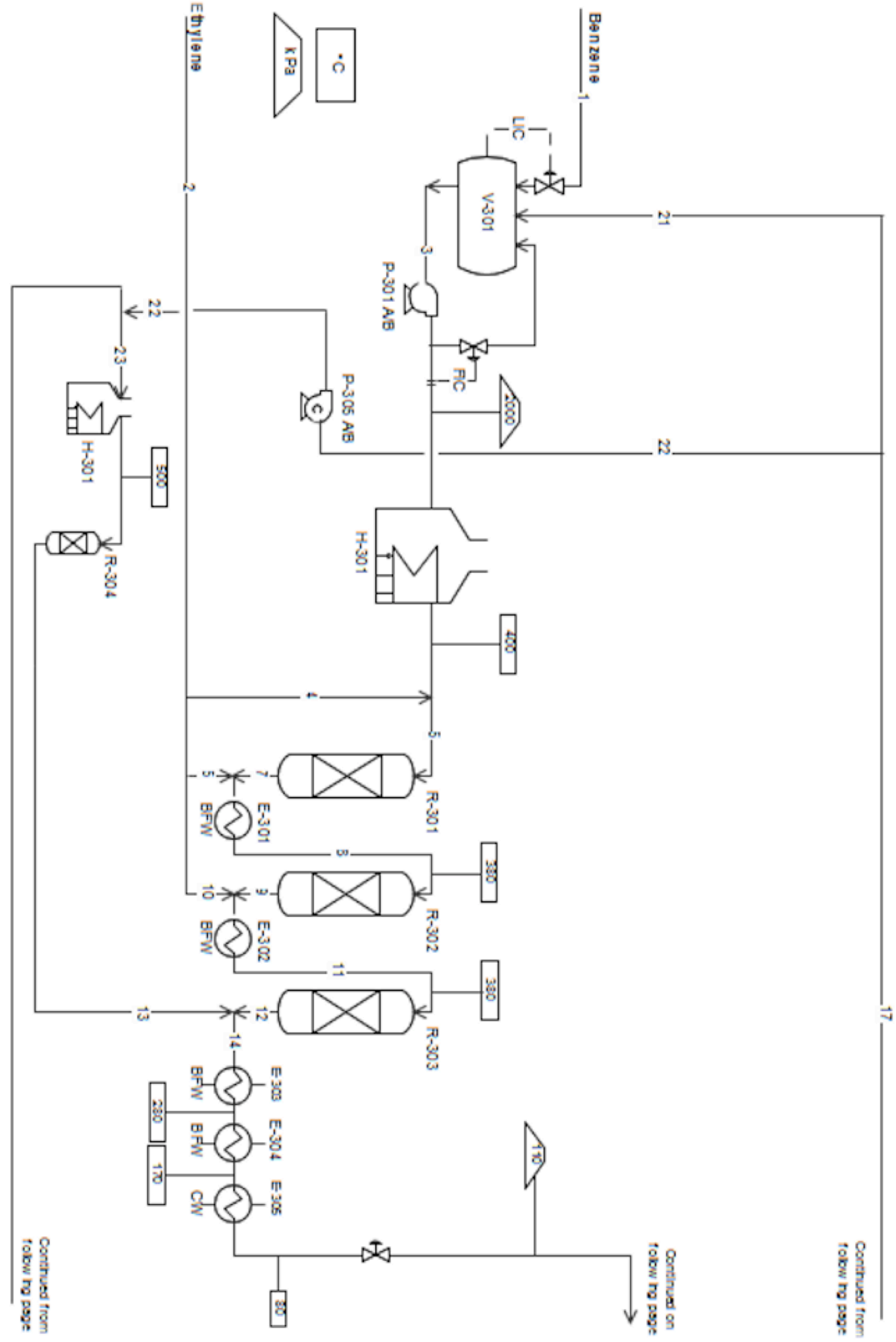
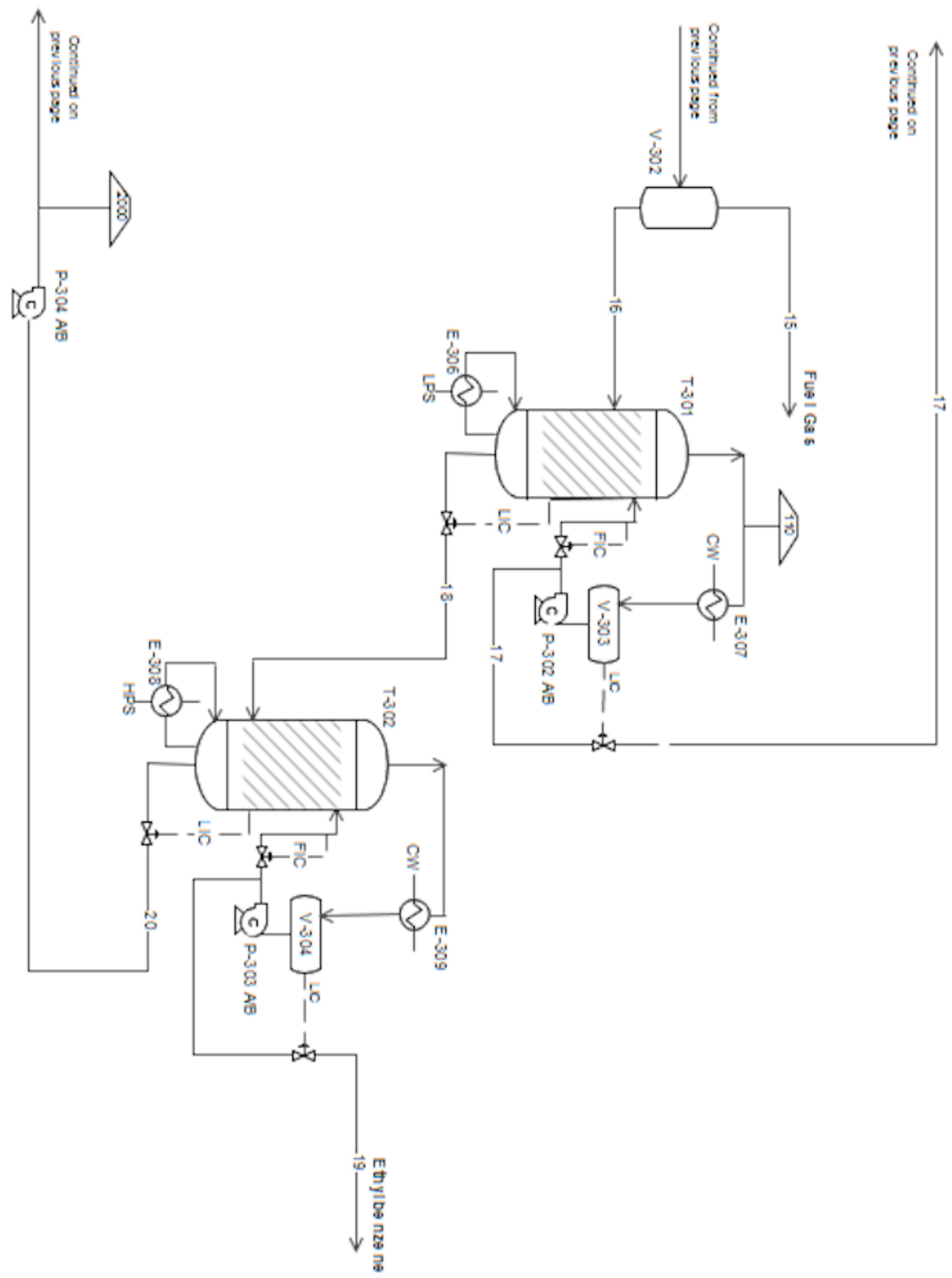


Figure 4: Process Flow Diagram of the Base Case Part 2



Stream Table of Base Case

Stream Name		**1**	**2**	**3**	**4**	**5**	**6**	**7**
Stream Description								
Phase		Liquid	Vapor	Liquid	Vapor	Vapor	Vapor	Vapor
Temperature	*C*	25	25	34.0	25	25	382.6	439.6
Pressure	*KPA*	110	2000	110	2000	2000	2000	1970
Rate	*KG-MOL/HR*	100	103	236.3	30.8	35.9	267.1	242.6
	KG/HR	7853.4	2890.5	18424.4	867.2	1011.7	19289.8	19289.8
Fluid Rates	*KG-MOL/HR*							
ETHYLENE			95.34	0.09	28.60	33.37	28.69	1.31
ETHANE			7.18	1.17	2.15	2.51	3.32	3.32
PROPYLEN				1.40			1.40	4.35
BENZENE		97		229.52			229.52	208.20
TOLUENE		3		3			3	0.04
Ethylbenzene				1.14			1.14	25.28
1,4-Diethylbenzene								0.15

Stream Name		**8**	**9**	**10**	**11**	**12**	**13**	**14**
Stream Description								
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	*C*	380	453.3	25	380	448.8	500	464.6
Pressure	*KPA*	1960	1945	2000	1935	1920	1988	1920
Rate	*KG-MOL/HR*	278.5	244.9	35.9	280.8	247.2	98.4	345.6
	KG/HR	20301.5	20301.5	1011.7	21313.2	21313.2	9304.7	30617.9
Fluid Rates	*KG-MOL/HR*							
ETHYLENE		34.68	1.00	33.37	34.37	0.85		0.85
ETHANE		5.83	5.83	2.51	8.34	8.34	0.35	8.69
PROPYLEN		4.35	4.40		4.40	4.40	0.42	4.81
BENZENE		208.20	174.86		174.86	141.73	38.79	180.52
TOLUENE		0.04						
Ethylbenzene		25.28	58.40		58.40	91.14	58.62	149.76
1,4-Diethylbenzene		0.15	0.40		0.40	0.79	0.17	0.96

Stream Name		**15**	**16**	**17**	**18**	**19**	**20**	**21**
Stream Description								
Phase		Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	*C*	73.6	73.6	50.1	142.9	139.3	149.4	50.1
Pressure	*KPA*	112.4	112.4	110	120	110	140	110
Rate	*KG-MOL/HR*	20.3	325.3	177.0	148.2	90.6	57.7	136.3
	KG/HR	1124.6	29499.7	13728.5	15764.8	9612.9	6151.9	10570.9
Fluid Rates	*KG-MOL/HR*							
ETHYLENE		0.74	0.11	0.11				0.09
ETHANE		7.18	1.51	1.51				1.17
PROPYLEN		3.00	1.81	1.81				1.40
BENZENE		8.19	172.33	172.10	0.20	0.18	0.023	132.52
TOLUENE								
Ethylbenzene		1.15	148.61	1.49	147.09	90.41	56.67	1.14
1,4-Diethylbenzene			0.96		0.96		0.96	

Stream Table of Base Case

Stream Name		**22**	**23**
Stream Description			
Phase		Liquid	Liquid
Temperature	*C*	50.1	114.0
Pressure	*KPA*	2000	2000
Rate	*KG-MOL/HR*	40.7	98.4
	KG/HR	3157.5	9309.4
Fluid Rates	*KG-MOL/HR*		
ETHYLENE		0.03	0.03
ETHANE		0.35	0.35
PROPYLEN		0.42	0.42
BENZENE		39.58	39.61
TOLUENE			
Ethylbenzene		0.34	57.01
1,4-Diethylbenzene			0.96

Process Description of the Optimized Plant:

The feed to the ethylbenzene plant consists of two streams. Benzene, which contains 10% toluene, is one feed stream, and ethylene, which contains 7% ethane, is the second feed stream. The benzene stream is first sent to a surge drum, V-301. The level controller on the surge drum guarantees that the proper amount of benzene is being sent into the surge drum to avoid one extreme of overfilling the drum to the other extreme of the drum becoming dry. The flow control valve ensures that the flow out of the surge drum remains consistent in order to avoid any problems downstream of lacking proper feed quantities. The flow of benzene out of the surge drum is then sent through a positive displacement pump, P-301, that discharges the benzene to a higher pressure of 2500 kPa. This high-pressure stream mixes with the recycled benzene from the tower. The stream of benzene then flows into the radiant section of the fired heater, H-301, where it is heated to the desired temperature of 293 °C for the reactor. This entails the reactor preparation section.

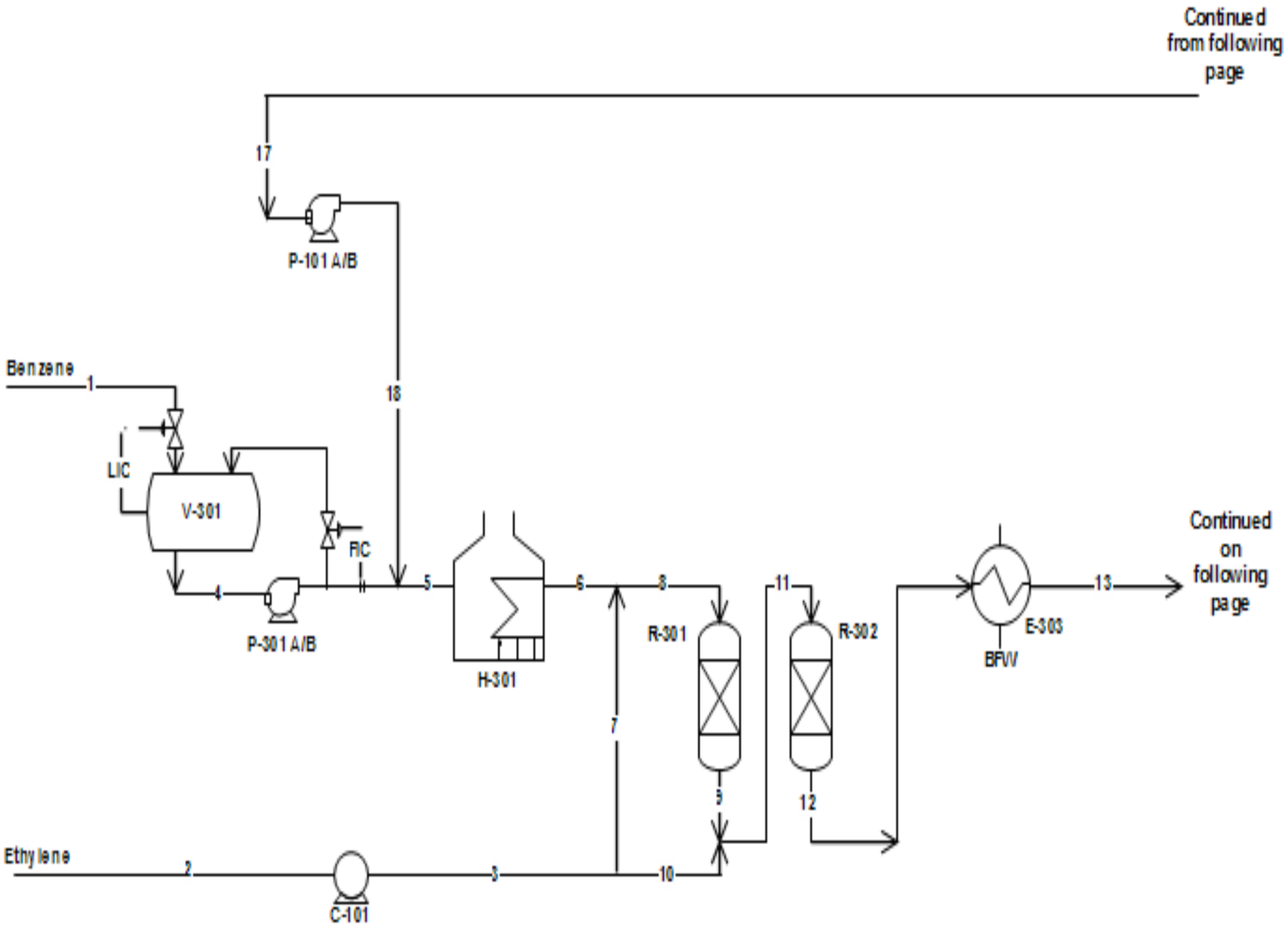
The heated stream of benzene enters the reactor section of the facility and is mixed with a small portion of the feed stream of ethylene. This mixture is sent to the reactor, R-301, at a low temperature and high pressure. The reactions that take place in the reactor are exothermic and exit the reactor at 311°C. This stream is then mixed with the rest of the ethylene feed and is sent into the second reactor, R-302. The product out of the second reactor is right below the catalyst maximum temperature of 500°C. The pressure drop across the reactors is minimum to ensure the proper products are formed from the four reactions. The exiting stream of the second reactor thus has essentially no ethylene but has the unreacted benzene. The products include ethylbenzene, diethylbenzene, propylene, and ethane.

The reactor exit stream is cooled using two heat exchangers E-303 and E-304 each producing steam. The first exchanger has boiler feed water in the cold process side and heats to high-pressure steam while cooling the reactor exit stream. The second exchanger is then used to make low-pressure steam while cooling the main process stream. The stream out of the second exchanger is partially condensed into a mixed stream at a temperature of 175°C. Both exchangers have the same pressure drop of 10 kPa. A valve is used to drop the pressure in the process stream down to the appropriate pressure in the separator of 600 kPa. The result of this valve also drops the temperature in the process stream down to 148°C. However, the stream remains a mixture of both liquid and vapor.

The separator, T-301, is used then to isolate the ethylbenzene from the rest of the feed stream in order to meet the specifications of the product. The light key in the column is the benzene and the heavy key is the ethylbenzene. The top half of the separator is cooled using cooling water in a condenser, E-307. The product of the condenser is a mixed stream that is separated in the reflux drum. The vapor portion is classified as fuel gas. The liquid stream out of the bottom of the reflux drum goes through a centrifugal pump, P-302, that increases the pressure enough to ensure the fluid has enough force behind it to get to the desired location. This stream is then split between the recycled benzene to the beginning of the reactor preparation section and the reflux to the column. The reflux to the column ensures the proper distillation is achieved by providing liquid on the trays. The recycle of benzene pressurizes in the positive displacement pump, P-101, to 2500 kPa before mixing with the fresh benzene feed.

The bottom of the column has the ethylbenzene and the minimal diethylbenzene. The reboiler, E-306, ensures that the product is separated to meet the criteria of 99.8% pure ethylbenzene product stream. The stream into the reboiler is liquid and the product out of the reboiler is at the same temperature but is a vapor stream. High-pressure steam is used to heat the reboiler. The liquid, product stream out of the column is cooled in the exchanger, E-105, using cooling water from a temperature of 218°C to the product specification of 139°C. This exchanger has a large pressure drop across it in order for the feed to be at the pressure of 110 kPa for the styrene plant. The ethylbenzene product is sent to the styrene plant where it is used accordingly.

Figure 5: Process Flow Diagram of the Optimized Plant Part 1



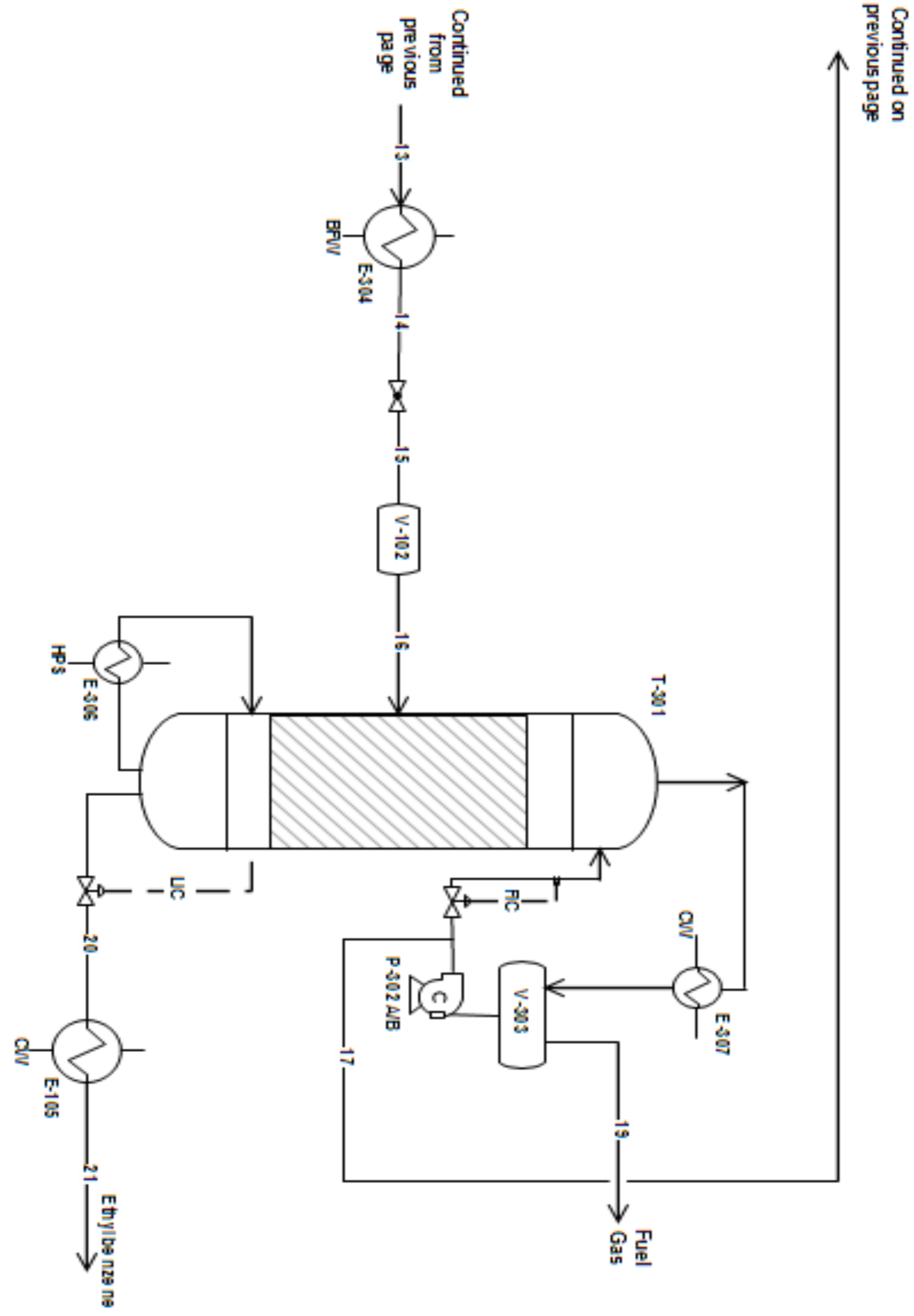


Figure 6: Process Flow Diagram of the Optimized Plant Part 2

Stream Table of Optimized Plant

Stream Name		**1**	**2**	**3**	**4**	**5**	**6**	**7**
Stream Description								
Phase		Liquid	Vapor	Vapor	Lliquid	Liquid	Vapor	Vapor
Temperature	*C*	25	25	39.5	25	36.3	293.5	39.5
Pressure	*KPA*	110	2000	2490	110	2500	2490	2490
Rate	*KG-MOL/HR*	91.7	107.1	107.1	91.7	165.4	165.4	19.3
	KG/HR	7287.7	3018.4	3018.4	7287.7	12561.4	12561.4	543.3
Fluid Rates	*KG-MOL/HR*							
ETHYLENE			99.56	99.56		0.0005		17.92
ETHANE			7.49	7.49		2.49	2.49	1.35
PROPYLEN						10.35	10.35	
BENZENE		82.49			82.49	143.4	143.4	
TOLUENE		9.17			9.17	9.17	9.17	
Ethylbenzene						0.014	0.014	
1,4-Diethylbenzene								

Stream Name		**8**	**9**	**10**	**11**	**12**	**13**	**14**
Stream Description								
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Mixed
Temperature	*C*	281.6	311.3	39.5	265.3	499.7	270	175
Pressure	*KPA*	2490	2475	2490	2475	2460	2450	2440
Rate	*KG-MOL/HR*	184.7	176.9	87.8	264.7	182.1	182.1	182.1
	KG/HR	13104.7	13104.7	2475.1	15579.8	15579.8	15579.8	15579.8
Fluid Rates	*KG-MOL/HR*							
ETHYLENE		17.92	4.31	81.64	85.95	0.003	0.003	0.003
ETHANE		3.84	3.84	6.14	9.99	9.99	9.99	9.99
PROPYLEN		10.35	16.13		16.13	19.52	19.52	19.52
BENZENE		143.4	141.3		141.32	62.14	62.14	62.14
TOLUENE		9.17	3.39		3.39			
Ethylbenzene		0.014	7.84		7.84	90.43	90.43	90.43
1,4-Diethylbenzene			0.0003		0.0003	0.0001	0.0001	0.0001

Stream Name		**15**	**16**	**17**	**18**	**19**	**20**	**21**
Stream Description								
Phase		Mixed	Mixed	Liquid	Liquid	Vapor	Liquid	Liquid
Temperature	*C*	149	149	50.3	50.8	50.3	218.7	139
Pressure	*KPA*	600	600	600	2500	600	610	110
Rate	*KG-MOL/HR*	182.1	182.1	73.8	73.8	17.7	90.6	90.6
	KG/HR	15579.8	15579.8	5272.6	5272.6	694.4	9612.9	9612.9
Fluid Rates	*KG-MOL/HR*							
ETHYLENE		0.003	0.003	0.0005	0.0005	0.002		
ETHANE		9.99	9.99	2.50	2.50	7.49		
PROPYLEN		19.52	19.52	10.37	10.37	9.16		
BENZENE		62.14	62.14	60.89	60.89	1.07	0.18	0.18
TOLUENE								
Ethylbenzene		90.43	90.43	0.014	0.014		90.41	90.41
1,4-Diethylbenzene		0.0001	0.0001				0.0001	0.0001

Manufacturing Costs:

Table 8: Summary of Manufacturing Costs per year

Cost of Utilities	$461,000
Cost of operating labor	$805,000
Cost of Raw Materials	$69.6 MM
COMd	$90.3 MM
Revenue	$108.4 MM

Table 9: Summary of Utilities Itemized

ID	Cooling/Heating Medium	Actual Usage GJ/hr.	Annual Cost(-)	Revenue (+)
E-303	BFW	8.79		$1.3 MM
E-304	BFW	0.69		$81,500
E-306	HPS	5.92	$873,000	----
E-307	CW	6.38	$18,800	----
E-105	CW	1.76	$5,200	
H-301	NG	10.1	$922,900	----
P-301			$3,700	----
P-101			$2,400	
C-101			$11,000	
P-302			$500	----

The values presented in Table 8 are calculated from our optimized facility. Our operating labor is calculated by assuming a basis of fourteen operators with a yearly salary of $57,500. The raw materials cost consists of benzene and ethylene. The catalyst cost is not included in Table 8 because it is not an annual cost. It must be replaced every four years due to the lifetime of the catalyst productivity. The cost to replace the catalyst every four years is $645,700. The manufacturing cost without depreciation (COMd) is calculated as a function of the total module cost, raw materials, utilities, and operating labor.

Investment and Equipment Summary:

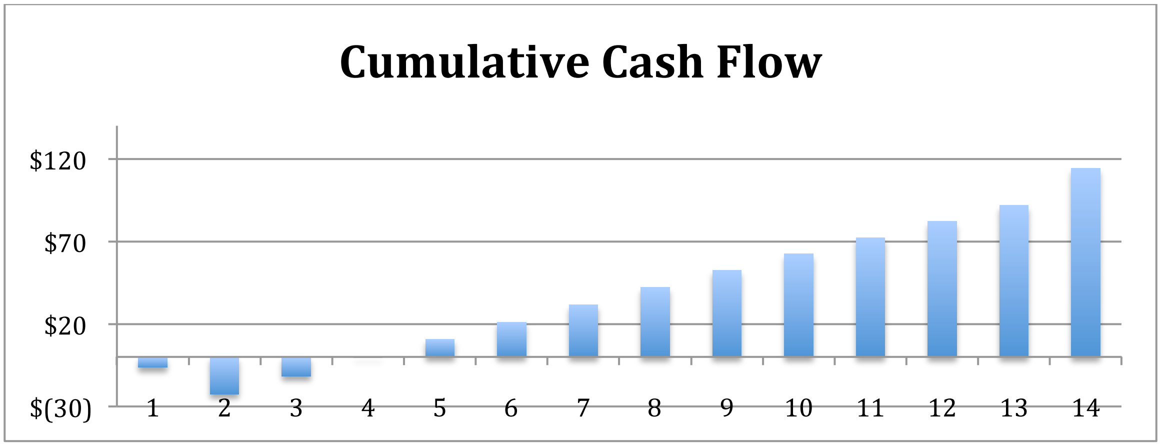


Figure 7: Cumulative Cash Flow, Non-discounted

Figure 7 describes the cash flow of the ethylbenzene production facility. This facility has a projected lifetime of 12 years and begins production at the beginning of year 3. The initial investment required to build a new facility will be $6.4 million for the first year and $4.3 million for the second year. The company will begin to see a return on the investment by the fifth year.

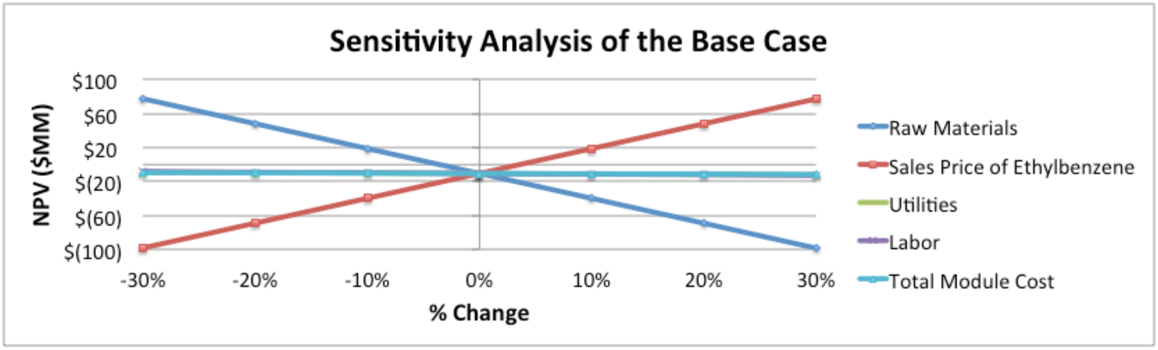


Figure 8: Sensitivity Analysis of the Base Case Plant

The sensitivity analysis as seen in Figure 8 shows that raw materials and revenue have the strongest effect on the overall net present value of the facility. The utilities, labor, and cost of equipment have minimal effect on the overall worth of the facility. For the facility to become more profitable, the raw materials cost need to be as low as possible while retaining the highest revenue of products.

All of the equipment prices are obtained from the pricing software CAPCOST and are scaled up to current prices using the most current CEPCI value of 574.3.

Table 10: Description of Heat Exchangers

	Pressure (barg)	Pressure (barg)	Area (m2)	Price	Type	MOC
E-303	25	41	241	$212,000	Floating Head	Carbon Steel
E-304	25	10	524	$256,000	Fixed, Sheet or U-Tube	Carbon Steel
E-306	6	5.16	52	$32,000	Fixed, Sheet or U-Tube	Carbon Steel
E-307	6	41	152	$160,000	Floating Head	Carbon Steel
E-101	6	5.16	4.56	$72,900	Fixed, Sheet or U-Tube	Carbon Steel

Table 10 illustrates that the exchanger's price is directly proportional to the pressure rating on the tube side and the type of exchanger. The material of construction is carbon steel because the pressure and temperatures being used do not exceed the limitations of carbon steel.

Table 11: Description of Fired Heater

	Pressure (barg)	Heat Duty (MJ/h)	Price	Type	MOC
H-301	25	10100	$1.7 MM	Process Heater	Carbon Steel

The fired heater is expensive to construct because of the pressure rating and the large size that is needed to adequately heat the feed stream into the reactor. Natural gas is used to fuel the heater in the radiant section. An efficiency of ninety percent is assumed while sizing the heater.

Table 12: Description of Pumps

	Pressure	Power (kW)	Price	Type	MOC	Number of Spares
P-301	25	5.55	$55,600	Positive Displacement	Carbon Steel	1
P-302	5	1	$26,200	Centrifugal	Carbon Steel	1
P-101	25	3.55	$48,200	Positive Displacement	Carbon Steel	1

The pumps are relatively inexpensive because the discharge pressure is not high enough to require an especially large pump. The efficiency of the pumps is high at 75%.

Table 13: Description of Compressor

	Power (kW)	Price	Type	MOC	Number of Spares
C-101	14.4	$83,100	Rotary	Carbon Steel	1

We recommend the addition of a compressor in the optimized facility in order to increase the pressure of the feed into the reactors. This is not present in the base case. It is assumed the compressor has an efficiency of 65%.

Table 14: Description of Distillation Tower

	Pressure	Height (m)	Diameter (m)	Price	Type	MOC
T-301	6.5	20.8	2	$545,000	37 Sieve Tray	Carbon Steel

The number of trays for the distillation tower includes the safety factor of 10% and also the 75% efficiency of the trays. The spacing between the trays is assumed to be half a meter and an additional three meters added to compensate for the top and bottom of the tower.

Table 15: Description of Vessels

	Pressure (barg)	Height (m)	Diameter (m)	Price	MOC
R-301	25	8.3	1.4	$476,000	Stainless Steel
V-301	25	5.6	1.87	$182,000	Carbon Steel
V-303	6	2.35	0.38	$23,300	Carbon Steel
R-302	25	13.2	2.4	$2.4 MM	Stainless Steel
V-102	6	3.31	1.1	$28,300	Carbon Steel

Each vessel is sized according to the residence time needed to ensure a safe process. For vessels feeding a heater, a residence time of thirty minutes is needed. Reflux vessels need a residence time of five minutes and vessels feeding a tower need approximately ten minutes. The material of choice, carbon steel, is appropriate for these vessels at the operating pressure and temperature because corrosion is not of great concern.

The reactor sizes are based on case studies to find the optimum length to minimize the amount of diethylbenzene and maximize the conversion of benzene. The reactors will need to be constructed of stainless steel due to the high operational temperatures and pressures.

Table 16: Process Conditions Matrix

Equipment	**High Temp**	**Low Temp**	**High Pressure**	**Low Pressure**	**Non Stoich. Feed**	**Comp**	**Exch.**	**Htr.**	**Valve**
R-301	x		x		x				
R-302	x		x		x				
R-303	x		x		x				
R-304	x		x		x				
V-301									
V-302									
V-303									
V-304									
T-301									
T-302									
E-301							x		
E-302							x		
E-303							x		
E-304									
E-305									
E-306									
E-307									
E-308									
E-309							x		
H-301									
P-301									
P-302									
P-303									
P-304									
P-305									
Valve before V-302									x

The Process Conditions Matrix as seen in Table 16 demonstrates the areas of special concern while optimizing the plant. Each piece of equipment is justified in using extreme conditions throughout the following the sections.

Top-down optimization process:

Topological optimization

The base case layout of reactors shows noticeable potential for improvement, with the key factor in this determination being the use of the packed bed reactor (PBR) R-304 to convert the undesired product, diethylbenzene, back into ethylbenzene. This process is done by reaction (3), which is relatively inefficient in that it has a higher activation energy than the desired reaction (1). This inefficiency is compounded by the fact that reactions (1), (2), and (3) take place in series, making the use of energy needed produce a mole of ethylbenzene through the undesired reactions a threefold increase over that which is required for each mole of ethylbenzene produced by (1). Problems from this scope on the molecular level translate to the big picture; therefore we saw it important to explore alterations that would decrease the production of diethylbenzene in the series PBRs R-301 to R-303. With the suggested catalyst change, reaction (2) – the ethylation of ethylbenzene forming undesired product – is significantly suppressed. Additionally, the new catalyst increases the rate of reaction (1). Table 17 illustrates the more favorable reaction kinetics obtained through the catalyst switch.

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

Table 17: Reaction Kinetics of New Catalyst

i	***E_I*** *kcal/kmol*	***k_{o,i}***	***a***	***b***	***c***	***d***	***e***
1	22500	1.50×10^6	1	0	0	1	0
2	22500	6.00×10^3	1	1	0	0	0
3	25000	7.80×10^6	0	0	0	1	1
4	20000	3.80×10^8	2	0	1	0	0

The units of r_i are $\frac{kmol}{s\,m^3}$ reactor, the units of C_i are $\frac{kmol}{m^3}$ gas, and the units of $k_{o,I}$ vary.

Since the new catalyst is so effective in improving the selectivity of ethylbenzene over diethylbenzene, our team was able to remove R-304 from the process. However, further inefficient topology of the base case process existed upstream from R-304 in the separation section of the plant, where distillation column T-302 was required to remove diethylbenzene from the product stream before it could be recycled to R-304. The decreased production of diethylbenzene and removal of R-304 left T-302 functioning only to refine the product stream from 14ppm DEB to the required maximum of 2ppm DEB. However, this particular constraint was met with parametric optimization of the upstream series of PBRs. Thus, we were also able to remove T-302.

The valve in stream 14 that drops the pressure in the separation section can be seen as a waste of energy. A reverse pump is a possible alternate. However the efficiency of reverse pumps are relatively low and the cost of the pump is higher than the valve. Therefore the large pressure drop across the valve is justified.

To conclude, the topology of the plant is heavily influenced by the type of catalyst used in the reaction process. Our team has found that the new catalyst allows for a far more optimal layout. This is because the amount of diethylbenzene produced is significantly decreased, therefore all process equipment involved in the conversion of this undesired product into ethylbenzene can be removed from the plant. This is a significant amount of equipment, and the savings in capital costs and operating costs outweigh the fact that the new catalyst is more expensive than the old one. These are the main topological improvements from the base case scenario that our team implements.

Parametric optimization

Our team investigates the effect of operating various process equipment at a range of temperatures and pressures. Since the rate of reaction is a function of concentration, and the reactions occur in the gas phase, increasing the pressure in the reactors results in a higher conversion of reactants, as shown in Figure 9. From this figure, we see that conversion asymptotically approaches approximately 55% as pressure rises above 2200 kPa.

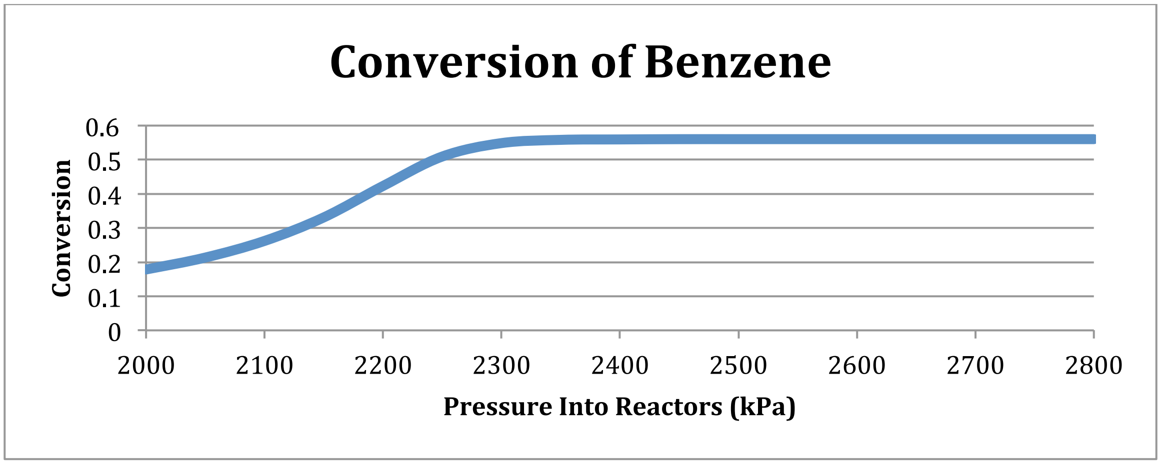


Figure 9: Pressure of the Reactors Directly Correlates to the Conversion of Benzene

We also consider the effect of reactor pressure on the selectivity of products. Figure 10 shows the production of diethylbenzene at various reactor inlet pressures.

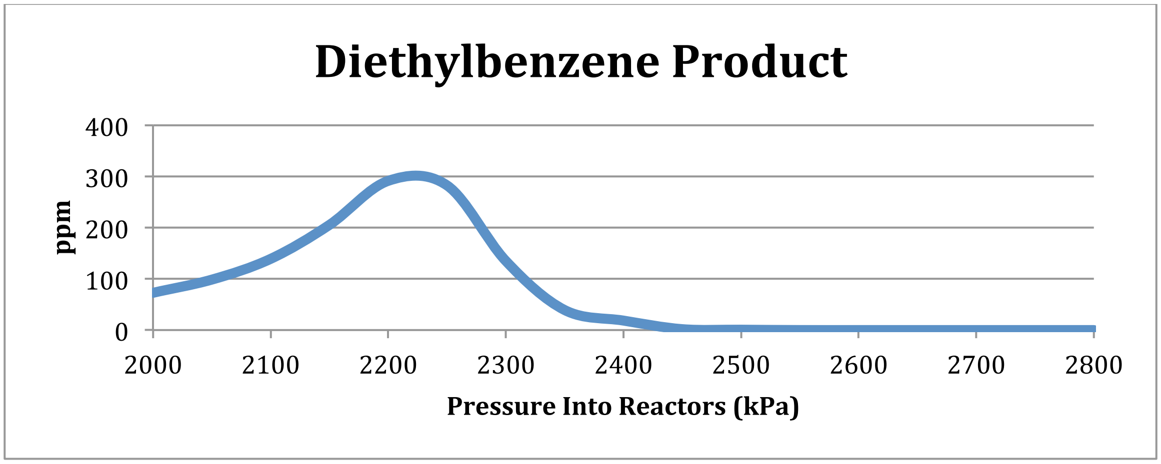


Figure 10: Pressure of the Reactor Affects the Amount of DEB

From figures 9 & 10, we determine that the domain of operating pressures that include both a maximum conversion of benzene and production rates of diethylbenzene below the 2ppm constraint is 2300-2500 kPa. The minimum of this domain is the optimal pressure at which the reactor should be operated.

Our team also ran a casestudy on the temperature effects of ethylbenzene production and diethylbenzene production. These results can be seen in Figures 11 & 12.

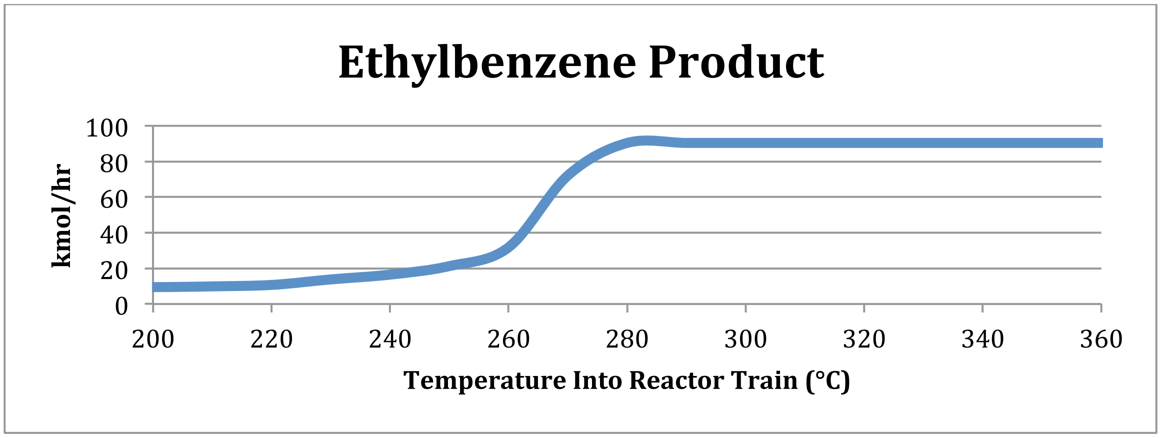


Figure 11: Temperature Into the Reactors Determines the Amount of Products Formed

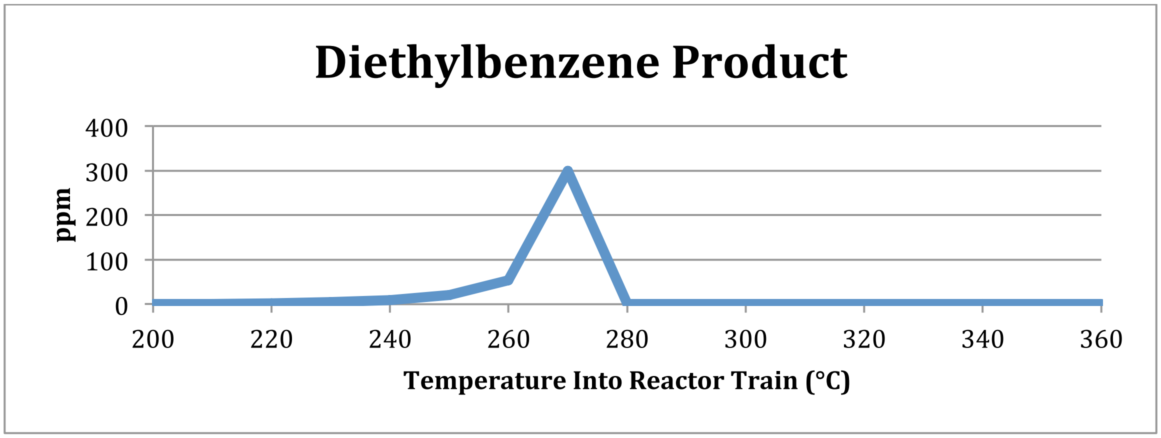


Figure 12: Inlet Temperature of the Reactors Directly Correspond with the DEB Production

Based on the results in these figures, we determine the optimal temperature of the reactor inlet stream to be 281°C. Since the reactor is adiabatic, there is a temperature gradient down the length of the reactor. To determine the total packed bed length that provides an optimal thermal profile, our team performed case studies to analyze the production of ethylbenzene and diethylbenzene, and these results are displayed in Figures 13 & 14. The optimum packed bed length in our optimized case is 11.9 meters. Our team models this as two Plug Flow Reactors without exceeding the maximum reactor temperature of 500 °C, and therefore negates the need for heat exchangers E-301 and E-302, which serve to control the temperature gradient along the longer packed bed length of PBRs R-301 through R-303 used in the base case.

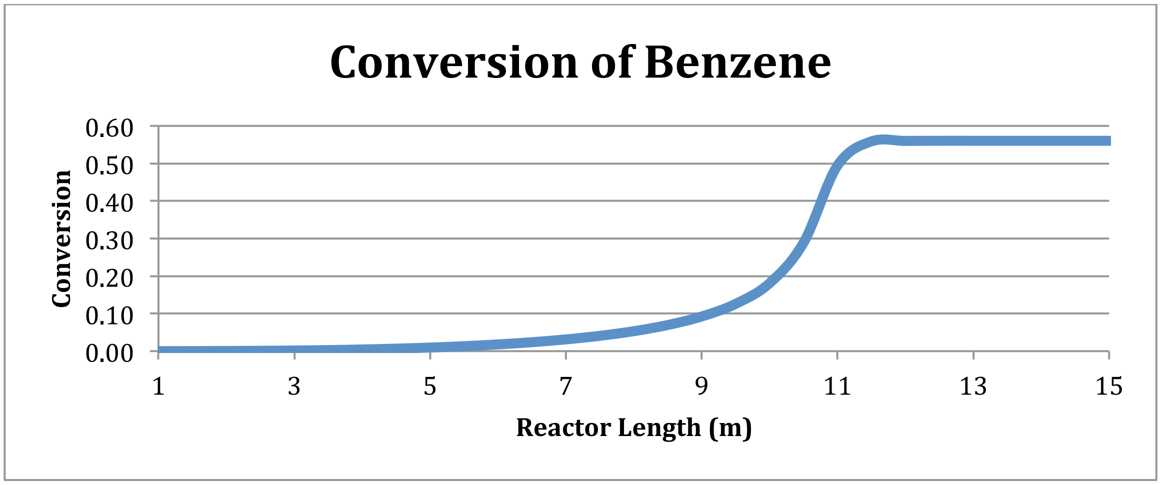


Figure 13: Reactor Length Effect on the Conversion of Benzene

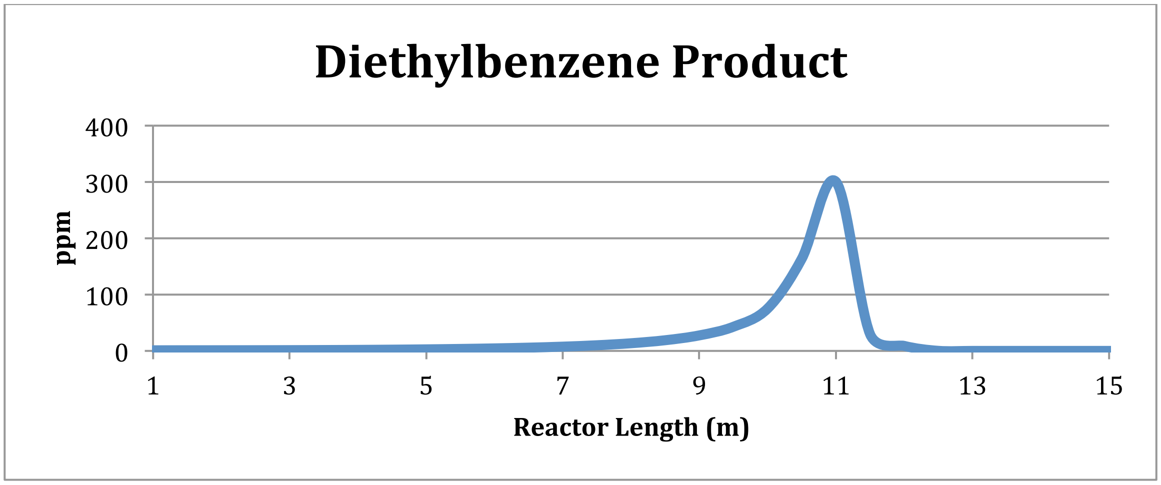


Figure 14: Reactor Length Effect on the Production of DEB

It is interesting to note that the rate of change of diethylbenzene production with respect to reactor inlet temperature has the same trend as it does with respect to reactor length (as can be seen by comparing Figures 11 & 12). This reinforces that the thermal profile of the reactor has a significant effect on the selectivity and should be central in optimizing the reactor section of the plant.

With regard to the separation section of the plant, the base case surrenders approximately 600 kg/hr of benzene to the fuel gas stream exiting flash vessel V-302. This is a loss of valuable raw material, so our team investigates how fuel gas can be separated more efficiently. We determine that removing V-302 and adding duty to the condenser on T-301 provides a viable alternative to this process. With non-condensable gases now being a significant fraction of the distillation column top products, the tower condenser is a partial condenser. However, when operating the tower at base case pressure and feed tray location, we still observe appreciable loss of benzene through the gas product of the partial condenser. By increasing the pressure of the tower feed, more benzene is forced into the liquid phase in the partial condenser and less is lost in the fuel gas stream. The ability to recycle more benzene lowers the expense of raw materials, which justifies the large pressure drop across the valve into the separator. Economically, the value of the benzene outweighs this loss of power and the additional costs associated with the condenser. With these changes in place, our team investigates the effect of the feed location on T-301. We determine that the optimal location is tray 12, where the combined duties of the re-boiler and condenser minimum.

Ultimately, parametric optimization allows our team to operate the process more efficiently by wasting less energy and raw materials. Further, we remove more process equipment and reduce the size of other equipment.

I. Other optimization

Purchasing a lower quality of benzene, with a mole fraction of 90/10 benzene to toluene at a cost of \$0.19/kg less than the higher quality benzene minimizes the cost of raw materials. Throughout the previously discussed optimization techniques, the process simulations utilize this new benzene feed. The effect of the lower purity benzene on the base case process can be seen in Table 18. The significant savings in raw materials made optimizing the process around this change a worthwhile investment of time. The process design fell within all constraints, and any additional process expenses resulting from the lower benzene quality were insignificant. Thus, our group emphasizes the importance of this feed change in any attempt to maximize the net present value of the project.

Table 18: Options Showed Significant Changes from the Base Case

Option	***Net Present Value***
Catalyst Change	\$4MM
Benzene Feed Change	\$28MM
Catalyst and Benzene Feed Change	\$34MM

Safety Concerns

Aside from the concern of the well being of the public, safety is a vital part of ensuring a plant is profitable. When an incident occurs, it slows production or can completely shut the process down for an extended period of time. People want to leave work in the same state that they came to work. Because of this, safety precautions are taken to ensure the protection of the workers and to maximize profit.

Flow control valves are heavily used in industry to guarantee that equipment has the adequate amount of materials. On the surge drum, a flow controller validates that the downstream process has continuous flow. If flow stops suddenly, the equipment will begin to run “dry” and have the tendency to break. Flow controllers in the distillation column validate that the condenser is sending the appropriate amount of reflux back into the column. If the column stops having the liquid reflux, the trays will consist of only vapor resulting in an inefficient separation. The tower might also over heat due to only having the hot vapors in the tower.

Level controllers are generally used when a product has a residence time in a piece of equipment. Surge drums have level controllers because if the drum overflows, production will cease and cleanup will have to take precedence over production. The bottoms product on a distillation column has a level controller. This controller ensures that the bottom of the column does not run dry and proper separation takes place. Sight glass can also serve as an immediate validation to what the level controller is predicting. Most columns and drums will have some sort of sight glass or other means of validation to check the reading on the level controller.

The reactors are adiabatic in order to avoid run away reactions from occurring. The temperature will increase in this case due to its kinetics being exothermic. However, after the reaction feed is terminated, the reactions can only take place until the feed runs out. This eliminates the run away reaction potential. Also the catalyst can only react to a certain extent and have a maximum temperature of 500°C. Once the catalyst "dies", there will be no conversion and the reactants will come and go in the same state.

Pressure relief valves need to be on all high-pressure equipment. If the equipment pressurizes past its capacity, it will more than likely explode. The pressure relief valve will open at a certain predetermined pressure and release into the atmosphere in order to avoid destruction of the equipment.

Safety should be the number one concern of a process. Utilizing these controls will help ensure the safety of the people and the equipment, which will ultimately maximize profitability.

Conclusions

Our group significantly increases the net present value of the ethylbenzene plant by choosing to optimize off of the options of changing the quality of the benzene and the change of catalyst. Although the feed change increases the amount of diethylbenzene, the catalyst change is more susceptible to the desired first reaction. Therefore both options of benzene feed change and catalyst change are selected.

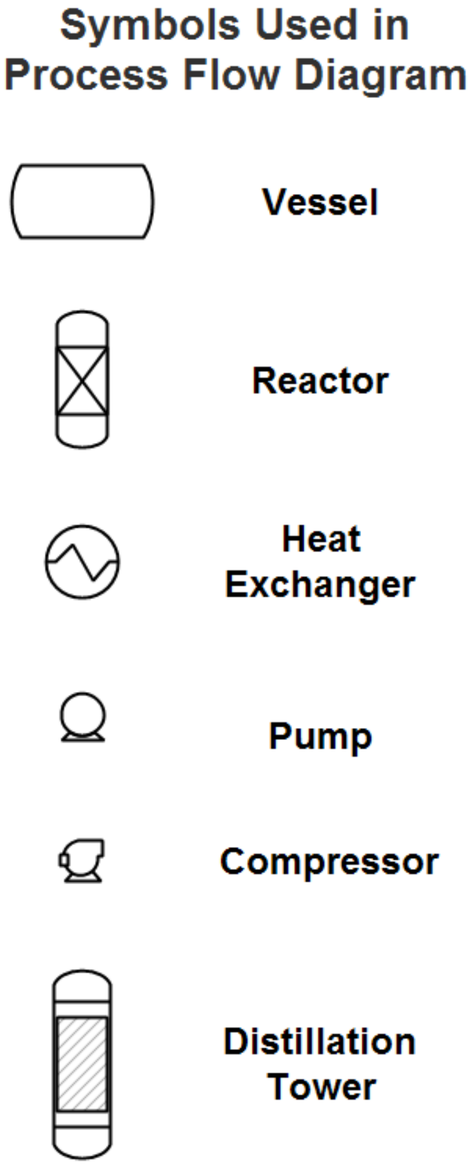
After implanting the changes, our team removes a significant amount of excess equipment. Because it is optimal to run this process at a high pressure, stainless steel is needed for the reactors. The optimal temperature and pressure for the entire process is found by the simulation program's case study and optimizer options.

We optimize the plant and successfully generate a net present value of $36 million. All of the specifications and constraints are met accordingly. The Ethylbenzene Production Plant is able to send 80,000 tonne/year of product to the Styrene Plant.

Recommendations

We decided that further investigation of separating the toluene for the benzene feed might be profitable in the lifetime of the plant. A case study looking into the effect on the equipment, the raw materials, and the net present value determines whether or not it is profitable. Further investigation into the removal of the fired heater may prove profitable to the plant. An analysis needs to be done in order to conserve the optimum conversion and selectivity. Removing the fired heater requires use of high-pressure steam as the initial heating for the reactor preparation. If the amount of high-pressure steam proves above the cost of the fired heater and cost of natural gas, then the removal of the fired heater is uneconomical. It is also recommended to further investigate the separator operating temperature and pressure. Although the amount of benzene lost as fuel gas is minimal, the amount of propylene that recycles with the benzene can be sold as fuel gas. Further investigation into this determines if there is a more economical way to operate the separator.

Nomenclature



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Invensys Systems. *Pro II Simulator*. Computer software.

"CAPCOST from the CD in Turton Et Al." *CAPCOST from the CD in Turton Et Al*. Web. 07 Dec. 2014.

Appendix

The following calculations are performed in order to properly size equipment to get the cost of each piece of equipment.

Sizing Heat Exchangers:

The latent heat and sensible heat areas combined are equivalent to the total area needed in an exchanger.

Sensible and Latent Area:

Find the amount of mass in the utility stream

$$m_{TOTAL} = \frac{Q_{TOTAL}}{\Delta H} \tag{1}$$

Solve for $Q_{SENSIBLE}$ by using the m_{TOTAL} from Equation (1)

$$Q_{SENSIBLE} = m_{TOTAL}\,\Delta H_{SENSIBLE} \tag{2}$$

Solve for Q_{LATENT} by using the m_{TOTAL} from Equation (1)

$$Q_{LATENT} = m_{TOTAL}\,\Delta H_{LATENT} \tag{3}$$

Find the intermediate temperature on the process stream

$$T_{INTERMEDIATE} = T_{HOT.IN} - \frac{Q_{LATENT}(T_{HOT.IN} - T_{HOT.OUT})}{Q_{TOTAL}} \tag{4}$$

Determine the Log Mean Temperature for both the Latent and Sensible areas

$$\Delta T_{LM} = \frac{(T_{HOT.IN} - T_{COLD.OUT}) - (T_{HOT.OUT} - T_{COLD.IN})}{\ln\left(\frac{T_{HOT.IN} - T_{COLD.OUT}}{T_{HOT.OUT} - T_{COLD.IN}}\right)} \tag{5}$$

Solve for the areas of each zone

$$A_{SENSIBLE} = \frac{Q_{SENSIBLE}}{UF_T \Delta T_{LM}} \qquad A_{LATENT} = \frac{Q_{LATENT}}{UF_T \Delta T_{LM}} \tag{6}$$

Add the Sensible Heat Area and Latent Heat Area for the Total Area

$$A_{TOTAL} = A_{SENSIBLE} + A_{LATENT} \tag{7}$$

For reboilers, the flux must be less than 31.5 $\frac{KW}{m^2}$

$$J = \frac{Q_{TOTAL}}{A_{TOTAL}} \tag{8}$$

Sizing Towers:

Find the minimal number of trays from the PRO II Simulator assuming perfect efficiency then solve for the optimal number of trays using a practical efficiency and a safety factor of 10%

$$N_{OPTIMAL} = \frac{N_{MIN}}{\eta}(1.1) \tag{9}$$

Solve for the height of the tower using the additional 3m for the top and bottom of the tower and 0.5m spacing between each tray

$$H_{TOWER} = 3 + 0.5(N_{OPTIMAL}-1) \tag{10}$$

Determine the volumetric velocity in the top and bottom of the tower where R is the reflux ratio acquired through PRO II and $\dot{m}$ is the mass flow rate and ρ_V is the density of the vapor

$$\dot{v} = \dot{m}\ \frac{(1+R)}{\rho_V} \tag{11}$$

Solve for the velocity in the top and bottom of the column using a range of F_S

$$F_S = \{1.2\text{-}1.5\}\ (\frac{m}{s})(\frac{kg}{m^3})^{0.5} \tag{12}$$

$$\nu = \frac{F_S}{\rho_v} \tag{13}$$

Solve for the Diameter of the tower using each velocity in Equation (12) and choose the biggest diameter as a safety precaution

$$D = (\frac{4\dot{v}}{\pi\ \nu})^{0.5} \tag{14}$$

Sizing Vessels:

Determine the proper residence time, τ, for the vessel based on the route downstream of the vessel. Get the volumetric flow rate, $\dot{v}$, of the outflowing liquid from the PRO II Simulation. For safety reasons only half the vessel needs to be full at all times.

$$V = 2\tau\dot{v} \tag{15}$$

The ratio of the length to the diameter must be approximately 3.

$$D = (\frac{4V}{3\pi})^{\frac{1}{3}} \tag{16}$$

$$L = \frac{4V}{\pi D^2} \tag{17}$$

Sample Calculations:

Heat Exchangers:

Given:

$Q_{TOTAL} = 1967\,\frac{MJ}{hr}$ $\Delta H = (2800 - 485)\,\frac{KJ}{kg}$ $T_{HOT.IN} = 423.9℃$

$T_{HOT.OUT} = 380℃$ $T_{COLD.IN} = 115℃$ $T_{COLD.OUT} = 254℃$ $U = 60\,\frac{W}{m^2℃}$

Calculations:

$$m_{TOTAL} = \frac{1967\frac{MJ}{hr}}{2315\frac{KJ}{kg}} * \frac{1000KJ}{MJ} = 849.7\,\frac{kg}{hr}$$

$$Q_{SENSIBLE} = 849.7\,\frac{kg}{hr} * \left(1101\,\frac{KJ}{kg} - 485\,\frac{KJ}{kg}\right) = 523.1\,\frac{MJ}{hr}$$

$$Q_{LATENT} = 849.7\,\frac{kg}{hr} * \left(2800\,\frac{KJ}{kg} - 1101\,\frac{KJ}{kg}\right) = 1443.6\,\frac{MJ}{hr}$$

$$T_{INTERMEDIATE} = 423.9℃ - \frac{1443.6\frac{MJ}{hr} * (423.9℃ - 380℃)}{1967\frac{MJ}{hr}} = 391.7℃$$

$$\Delta T_{LM} = \frac{(423.9℃ - 254℃) - (391.7℃ - 254℃)}{\ln\left(\frac{423.9℃ - 254℃}{391.7℃ - 254℃}\right)} = 131.8℃$$

$$A_{SENSIBLE} = \frac{523.1\frac{MJ}{hr}}{60\,\frac{W}{m^2℃} * 0.9 * 219℃} = 12.3m^2$$

$$A_{LATENT} = \frac{1443.6\frac{MJ}{hr}}{60\,\frac{W}{m^2℃} * 131.8℃} = 50.7m^2$$

$$A_{TOTAL} = 12.3m^2 + 50.7m^2 = 63m^2$$

Towers:

Given:

$N_{MIN} = 11.5 \quad \varepsilon = 0.75 \quad \dot{m} = 9538\,\frac{kg}{hr} \quad \rho_V = 3.41\,\frac{kg}{m^3} \quad R = 0.66$

Calculations:

$$N_{OPTIMAL} = \frac{11.5}{.75} * 1.1 * 2 = 34\ trays$$

$$H_{TOWER} = 3 + 0.5 * (34 - 1) = 19.5m$$

$$\dot{v} = 9538\ \frac{kg}{hr} * \frac{(1+0.66)}{3.41\frac{kg}{m^3}} = 1.2\,\frac{m}{s}$$

$$v = \frac{\{1.2-1.5\}\,(\frac{m}{s})(\frac{kg}{m^3})^{0.5}}{3.41\frac{kg}{m^3}} = 0.65\,\frac{m}{s}\ to\ 0.81\,\frac{m}{s}$$

$$D = \frac{4*1.2\frac{m}{s}}{\pi*0.65\frac{m}{s}\ to\ 0.81\frac{m}{s}}^{0.5} = 1.42\ m\ to\ 1.59\ m$$

Vessels:

Given:

$\tau = 10min \quad \dot{v} = 30\frac{m^3}{hr}$

Calculations:

$$V = 2 * 10min * 30\,\frac{m^3}{hr} = 10m^3$$

$$D = \left(\frac{4*10m^3}{3\pi}\right)^{\frac{1}{3}} = 1.62m$$

$$L = \frac{4*10m^3}{\pi*(1.62m)^2} = 4.85m$$

The following equations are the general equations needed to calculate the net present value of a plant after the equipment has been sized and priced.

Cost of Utilities:

For heat exchangers the total duty needed and the price of boiler feed water is subtracted from the amount of steam being produced.

$$\$\text{Utility}_{\text{EXCHANGER}} = Q\frac{\$_{Steam}}{Energy} - Q\frac{\$_{BFW}}{Energy} \tag{18}$$

For pumps and compressors the work, W, is calculated in PRO II

$$\$\text{Utility}_{\text{PUMP}} = W\frac{\$}{Energy} \tag{19}$$

Cost of Operating Labor:

The cost of operating labor is based upon an annual average salary of \$57,500. P is the number of processing steps and N_{np} is the number of nonparticulate processing steps. N_{OL} is the number of operators per shift.

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \tag{20}$$

$$C_{OL} = \$57500\ N_{OL} \tag{21}$$

Cost of Manufacturing:

The Fixed Capital Investment, FCI, Cost of Operating Labor from Equation 21, Cost of Utilities from Equation 18/19, and Cost of Raw Materials, C_{RM}, all add together for the Cost of Manufacturing without depreciation.

$$COM_d = 0.18FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{RM}) \tag{22}$$

Net Present Value:

The net cash flow is calculated by subtracting the total cost from the revenue generated yearly. The total cost includes cost of utilities, operating labor, and manufacturing. It also includes taxes, building costs, working capital, and catalyst costs. The Capital Investment is depreciated using MACRS 7 year category. Taxation rate is 45% per year.

$$\text{Others} = 0.18\text{FCI} + 1.73C_{OL} + 0.23(C_{RM} + C_{UT}) \tag{23}$$

$$\text{Taxable Income} = \text{Revenue} - C_{RM} - C_{OL} - C_{UT} - \text{Others} - \text{Catalyst} - \text{Depreciation} \tag{24}$$

$$\text{Taxes} = 0.45(\text{Taxable Income}) \tag{25}$$

$$\text{Working Capital} = \frac{1}{6}C_{RM} + \frac{1}{4}C_{OL} \tag{26}$$

The net cash flow for each year, N, must then be brought to present value assuming a MARR value of 12%.

$$\text{Present Value} = \frac{Cash\ Flow}{1.12^{N}} \tag{27}$$

$$\text{Net Present Value} = \Sigma\ \text{Present Value} \tag{28}$$

Figure 15: Pro II Simulation of Base Case Plant

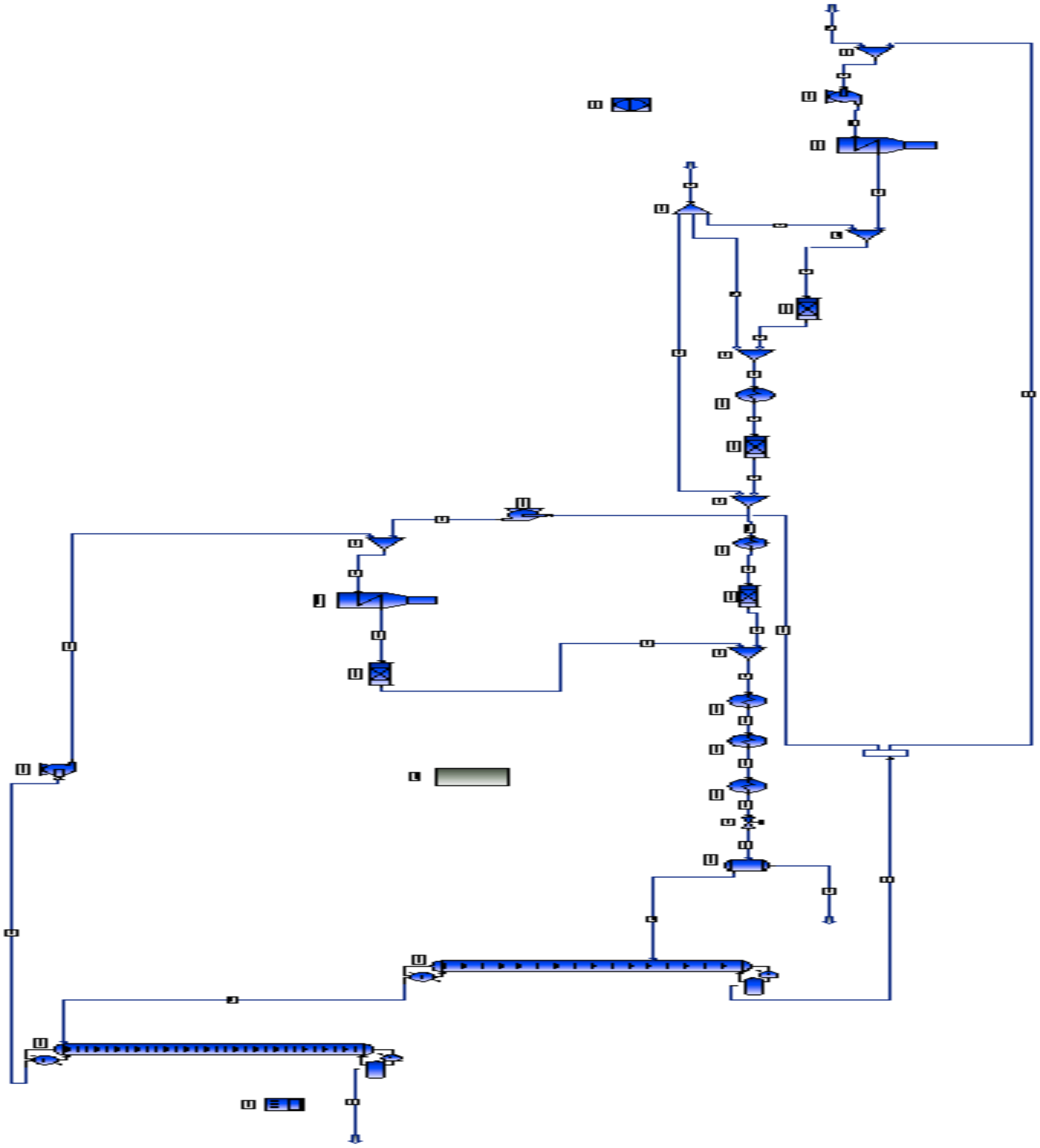

Table 18: Pro II Simulator Base Case Stream Table

Stream Name		1	2	3	3B	3C	4	5
Stream Description								
Phase		Liquid	Vapor	Liquid	Liquid	Vapor	Vapor	Vapor
Temperature	C	25.0	25.0	34.0	34.3	400.0	25.0	25.0
Pressure	KPA	110	2000	110	2000	2000	2000	2000
Enthalpy	M*KJ/HR	0.317	0.929	1.050	1.091	20.176	0.279	0.325
Molecular Weight		78.53	28.19	77.96	77.96	77.96	28.19	28.19
Mole Fraction Vapor		0	1	0	0	1	1	1
Mole Fraction Liquid		1	0	1	1	0	0	0
Rate	KG-MOL/HR	100	102.52	236.31	236.31	236.31	30.76	35.88
Fluid Rates	KG-MOL/HR							
ETHYLENE			95.343	0.087	0.087	0.087	28.603	33.370
ETHANE			7.176	1.166	1.166	1.166	2.153	2.512
PROPYLEN				1.395	1.395	1.395		
BENZENE		97		229.519	229.519	229.519		
TOLUENE		3		3	3	3		
EBENZENE				1.144	1.144	1.144		
14EZ								

Stream Name		6	7	8A	8	9	10	11A
Stream Description								
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	C	382.6	439.6	418.8	380.0	453.3	25.0	433.2
Pressure	KPA	2000	1970	1970	1960	1945	2000	1945
Enthalpy	M*KJ/HR	20.454	22.989	23.314	21.485	24.963	0.325	25.288
Molecular Weight		72.23	79.50	72.89	72.89	82.90	28.19	75.91
Mole Fraction Vapor		1	1	1	1	1	1	1
Mole Fraction Liquid		0	0	0	0	0	0	0
Rate	KG-MOL/HR	267.07	242.64	278.53	278.53	244.89	35.88	280.78
Fluid Rates	KG-MOL/HR							
ETHYLENE		28.690	1.309	34.679	34.679	1.004	33.370	34.374
ETHANE		3.319	3.319	5.830	5.830	5.830	2.512	8.342
PROPYLEN		1.395	4.354	4.354	4.354	4.395		4.395
BENZENE		229.519	208.200	208.200	208.200	174.861		174.861
TOLUENE		3.000	0.042	0.042	0.042			
EBENZENE		1.144	25.277	25.277	25.277	58.404		58.404
14EZ			0.145	0.145	0.145	0.398		0.398

Stream Name		11	12	13	14	14B	14C	14D
Stream Description								
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid
Temperature	C	380.0	448.8	500.0	464.6	280.0	170.0	80.0
Pressure	KPA	1935	1920	1988	1920	1910	1900	1890
Enthalpy	M*KJ/HR	22.602	26.070	12.580	38.650	25.398	10.191	4.424
Molecular Weight		75.91	86.20	94.61	88.59	88.59	88.59	88.59
Mole Fraction Vapor		1	1	1	1	1	0	0
Mole Fraction Liquid		0	0	0	0	0	1	1
Rate	KG-MOL/HR	280.78	247.25	98.35	345.60	345.60	345.60	345.60
Fluid Rates	KG-MOL/HR							
ETHYLENE		34.374	0.849	0.003	0.852	0.852	0.852	0.852
ETHANE		8.342	8.342	0.348	8.690	8.690	8.690	8.690
PROPYLEN		4.395	4.395	0.417	4.812	4.812	4.812	4.812
BENZENE		174.861	141.729	38.794	180.524	180.524	180.524	180.524
TOLUENE								
EBENZENE		58.404	91.142	58.616	149.758	149.758	149.758	149.758
14EZ		0.398	0.792	0.173	0.965	0.965	0.965	0.965

Stream Name		14E	15	16	17	18	19	20
Stream Description								
Phase		Mixed	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	73.4	73.6	73.6	40.6	142.9	139.3	149.4
Pressure	KPA	110	112	112	110	120	110	140
Enthalpy	M*KJ/HR	4.424	0.581	3.843	0.952	4.174	2.470	1.716
Molecular Weight		88.59	55.52	90.65	77.54	106.31	106.11	106.62
Mole Fraction Vapor		0.06	1	0	0	0	0	0
Mole Fraction Liquid		0.94	0	1	1	1	1	1
Rate	KG-MOL/HR	345.60	20.26	325.34	177.03	148.25	90.59	57.66
Fluid Rates	KG-MOL/HR							
ETHYLENE		0.852	0.738	0.113	0.113			
ETHANE		8.690	7.176	1.514	1.514			
PROPYLEN		4.812	3.000	1.812	1.812			
BENZENE		180.524	8.193	172.330	172.103	0.200	0.177	0.023
TOLUENE								
EBENZENE		149.758	1.146	148.611	1.486	147.087	90.415	56.672
14EZ		0.965	0.001	0.963		0.962		0.962

Stream Name		20B	21	22A	22	23	23B
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Vapor
Temperature	C	150.0	40.6	40.6	40.9	114.0	500.0
Pressure	KPA	2000	110	110	2000	2000	1990
Enthalpy	M*KJ/HR	1.732	0.733	0.219	0.226	1.958	12.583
Molecular Weight		106.62	77.54	77.54	77.54	94.59	94.59
Mole Fraction Vapor		0	0	0	0	0	1
Mole Fraction Liquid		1	1	1	1	1	0
Rate	KG-MOL/HR	57.66	136.31	40.72	40.72	98.37	98.37
Fluid Rates	KG-MOL/HR						
ETHYLENE			0.087	0.026	0.026	0.026	0.026
ETHANE			1.166	0.348	0.348	0.348	0.348
PROPYLEN			1.395	0.417	0.417	0.417	0.417
BENZENE		0.023	132.519	39.584	39.584	39.607	39.607
TOLUENE							
EBENZENE		56.672	1.144	0.342	0.342	57.014	57.014
14EZ		0.962				0.962	0.962

Figure 16: Pro II Simulation of Optimized Plant

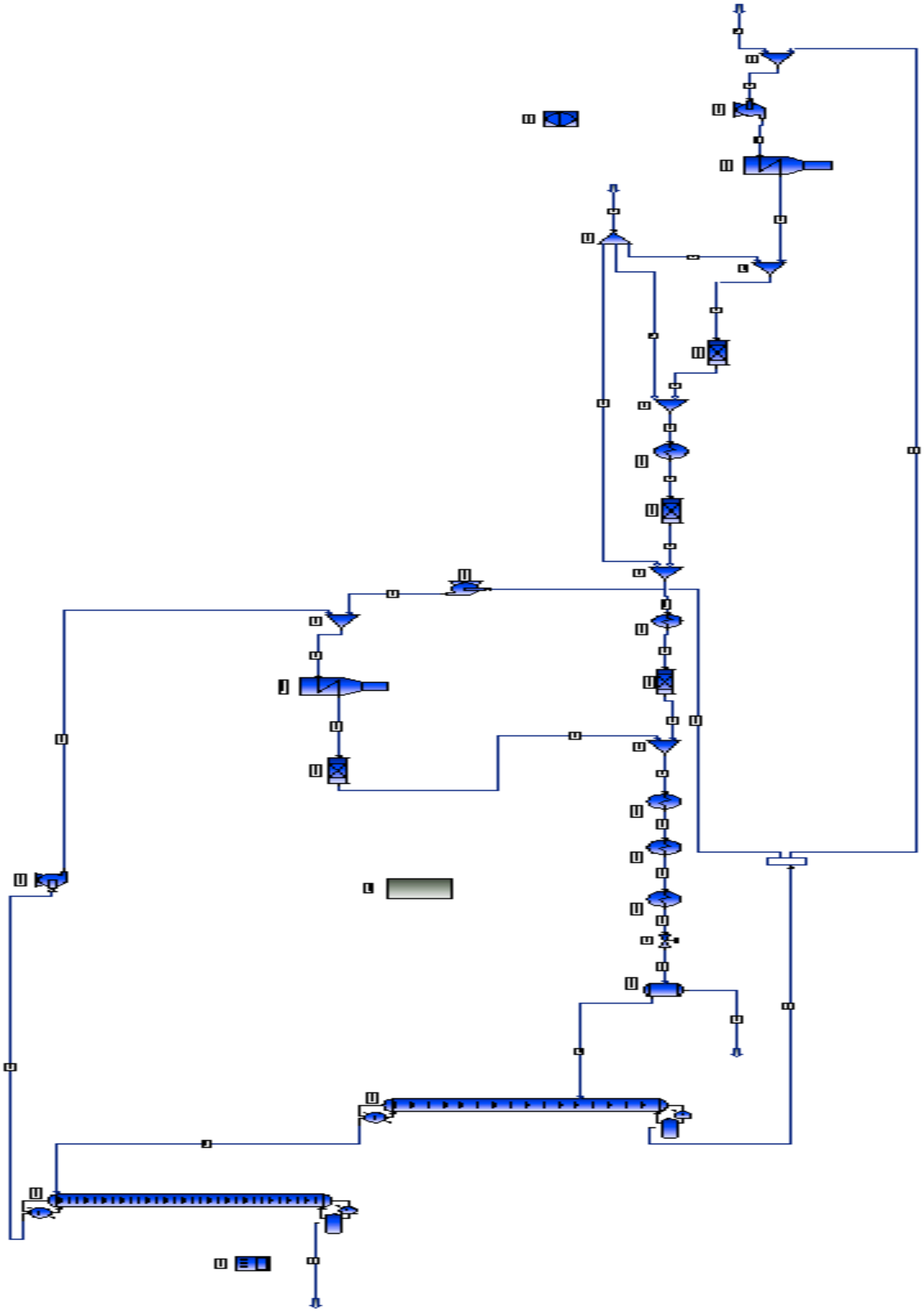

Table 19: Pro II Simulator Optimized Stream Table

Stream Name		1	2	3	4	5	6	7
Stream Description								
Phase		Liquid	Vapor	Vapor	Liquid	Liquid	Vapor	Vapor
Temperature	C	25	25	39.54	25.35	36.37	293.50	39.54
Pressure	KPA	110	2000	2490	2500	2500	2490	2490
Enthalpy	M*KJ/HR	0.30	0.97	1.02	0.32	0.80	10.78	0.18
Molecular Weight		79.52	28.19	28.19	79.52	75.91	75.91	28.19
Mole Fraction Vapor		0	1	1	0	0	1	1
Mole Fraction Liquid		1	0	0	1	1	0	0
Rate	KG-MOL/HR	91.65	107.08	107.08	91.65	165.45	165.45	19.27
Fluid Rates	KG-MOL/HR							
ETHYLENE			99.581	99.581				17.925
ETHANE			7.495	7.495		2.495	2.495	1.349
PROPYLEN					0.000	10.376	10.376	
BENZENE		82.485			82.485	143.400	143.400	
TOLUENE		9.165			9.165	9.165	9.165	
EBENZENE						0.014	0.014	
14EZ								

Stream Name		8	9	10	11	12	13	14
Stream Description								
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Mixed
Temperature	C	281.58	311.29	39.54	265.29	499.77	270.00	175.00
Pressure	KPA	2490	2475	2490	2475	2460	2450	2440
Enthalpy	M*KJ/HR	10.97	11.80	0.84	12.64	21.24	12.45	5.48
Molecular Weight		70.93	74.07	28.19	58.85	85.54	85.54	85.54
Mole Fraction Vapor		1	1	1	1	1	1	0.003
Mole Fraction Liquid		0	0	0	0	0	0	0.997
Rate	KG-MOL/HR	184.72	176.89	87.80	264.70	182.11	182.11	182.11
Fluid Rates	KG-MOL/HR							
ETHYLENE		17.925	4.316	81.656	85.972	0.003	0.003	0.003
ETHANE		3.844	3.844	6.146	9.984	9.984	9.984	9.984
PROPYLEN		10.376	16.156		16.148	19.532	19.532	19.532
BENZENE		143.400	141.350		141.369	62.168	62.168	62.168
TOLUENE		9.165	3.386		3.385			
EBENZENE		0.014	7.843		7.840	90.426	90.426	90.426
14EZ			0.0003		0.0003	0.0001	0.0001	0.0001

Stream Name		16	17	18	19	20	21
Stream Description							
Phase		Mixed	Liquid	Liquid	Vapor	Liquid	Liquid
Temperature	C	148.94	50.30	50.82	50.30	218.67	139.00
Pressure	KPA	600	600	2500	600	610	110
Enthalpy	M*KJ/HR	5.48	0.47	0.49	0.32	4.23	2.46
Molecular Weight		85.54	71.43	71.43	39.19	106.11	106.11
Mole Fraction Vapor		0.274	0	0	1	0	0
Mole Fraction Liquid		0.726	1	1	0	1	1
Rate	KG-MOL/HR	182.11	73.80	73.80	17.72	90.59	90.59
Fluid Rates	KG-MOL/HR						
ETHYLENE		0.003			0.002		
ETHANE		9.984	2.495	2.495	7.489		
PROPYLEN		19.532	10.376	10.376	9.156		
BENZENE		62.168	60.915	60.915	1.073	0.180	0.180
TOLUENE							
EBENZENE		90.426	0.014	0.014	0.000	90.412	90.412
14EZ		0.0001				0.0001	0.0001