Spring 5-12-2023

An Analysis of the Production of Pharmaceutical-Grade Acetone via the Dehydrogenation of Isopropanol (IPA)

Jordan Desplas

Recommended Citation

Desplas, Jordan, "An Analysis of the Production of Pharmaceutical-Grade Acetone via the Dehydrogenation of Isopropanol (IPA)" (2023). *Honors Theses*. 2911.
https://egrove.olemiss.edu/hon_thesis/2911

AN ANALYSIS OF THE PRODUCTION OF PHARMACEUTICAL-GRADE ACETONE VIA THE DEHYDROGENATION OF ISOPROPANOL (IPA)

by
Jordan Michael Desplas

Oxford
May 2023

Approved By:

Joanna Harrelson
Advisor: Professor Joanna Harrelson

Reader: Professor Adam Smith

Reader: Professor Mike Gill

ABSTRACT

JORDAN MICHAEL DESPLAS: An Analysis of The Production of Pharmaceutical-Grade Acetone via the Dehydrogenation of Isopropanol (IPA)

The production of 99.9 wt% acetone from isopropanol in Unit 1100 is designed to start up in 2025 and operate for 12 years after startup. The engineering team was tasked with designing the process, creating an economic model, and optimizing the net present value (NPV). The process was simulated in AVEVA PRO/II Simulation for the design process, and the economic analysis was estimated in Microsoft Excel. Parametric and topological optimization was performed linearly on the unit operations in the process. The NPV was improved by \$14M from a base case of \$122M to an optimized case of \$136M. The project is recommended to continue for more in-depth economic analysis and further optimization. Furthermore, the safety, environmental, and societal impacts from the facility will be analyzed before the plant is constructed. Additionally, a fluidized bed reactor was then simulated in PRO/II and optimized based on selectivity of the desired product, acetone, to the raw material, isopropanol. The optimized reactor is discussed after the isopropanol to acetone optimization.

Table of Contents

List of Figures

List of Abbreviations

IPA	Isopropyl alcohol
PFR	Plug flow reactor
wt%	Percentage by weight
NPV	Net present value of project
O_2	Oxygen
BPA	Bisphenol A

Introduction

In the isopropyl alcohol (IPA) to acetone process, both water and IPA are fed through a series of heat exchangers into a plugged flow reactor (PFR) where the endothermic reaction of the dehydrogenation of IPA occurs. When the IPA is heated, acetone and hydrogen are formed, as seen in equation 1.

$$\underset{\text{IPA}}{(CH_3)_2CHOH} \quad \underset{2}{\overset{1}{\rightleftarrows}} \quad \underset{\text{acetone}}{(CH_3)_2CO} \quad + \quad \underset{\text{hydrogen}}{H_2} \qquad \text{(Eqn. 1)}$$

From there, the reactor effluent is sent into an absorber to separate the hydrogen, sold as fuel gas, from organics. The organics and water are then sent to a distillation column where the acetone is separated into 99.9 wt% product purity. The remaining components are then sent to a second distillation tower that separates into a bottom wastewater stream containing 0.1 wt% organics, and the distillate is recycled into the reactor for the purpose of reacting any unused IPA (Harrelson, 2023).

A base-case model was constructed based on information that was readily available. However, there were areas capable of optimization to improve the initial net present value (NPV) of $122 million. Optimization variables kept both safety and environmental factors in mind, as well as global, social, and economic factors. There was an option for a low temperature catalyst or a high temperature catalyst. It was determined that due to the large recycle in the low temperature catalyst reactor, the high temperature catalyst provided the highest NPV. To further optimize this process, variables such as the reactor section conditions, the separation section conditions, the tower sequencing, and heat integration were investigated. It was determined that increasing the reactor temperature and pressure, as well as decreasing the number of reactor tubes produced the greatest gains in NPV for the reactor section. In the separations section, the greatest gain in NPV was from increasing the water flowrate in the absorber. These optimization areas resulted in an ultimate NPV of $136 million, which is an 11.5% increase from the base-case model. It is recommended to continue with the planning to construct this plant since there is a large margin of profitability. The engineers are seeking approval to dive deeper into the economic analysis to get a more accurate assessment of the profitability of this project.

Initial Recommendations

The project should continue because of the large return on investment. The NPV of the project was $136 million. Additionally, the process can produce the 99.9 wt% acetone in a safe and environmentally friendly manner. The next step would be to further investigate the economics of the project to get a more accurate NPV. Another plan of action is to further investigate the impact each variable has on one another. In this report, the variables were considered in a linear fashion. It would be beneficial to modify these variables in tandem.

Optimized Design

From the previous optimization cycles, it was determined that the high temperature catalyst was the most profitable in comparison to both low temperature catalyst scenarios. From there, the reactor was optimized to increase the conversion, which will decrease the duty on the last distillation tower. It was found that increasing temperature and then pressure increased the conversion. In addition, while increasing the tube number has the potential to increase the conversion, the reactor produces the highest NPV with fewer tubes, as there is less catalyst needed to fill the reactor. Ultimately operating conditions at 460°C, 230 tubes, and 4.5 bar are recommended.

After the reactor, the first tower was optimized, as it was observed that increasing the water flowrate helped to increase the recovery of acetone. The operating water flowrate recommended is 153 kmol/hr. In Figure 1, the effects each of these variables had on the NPV can be observed. There are still additional areas for optimization to be discussed further in the latter sections of this report.

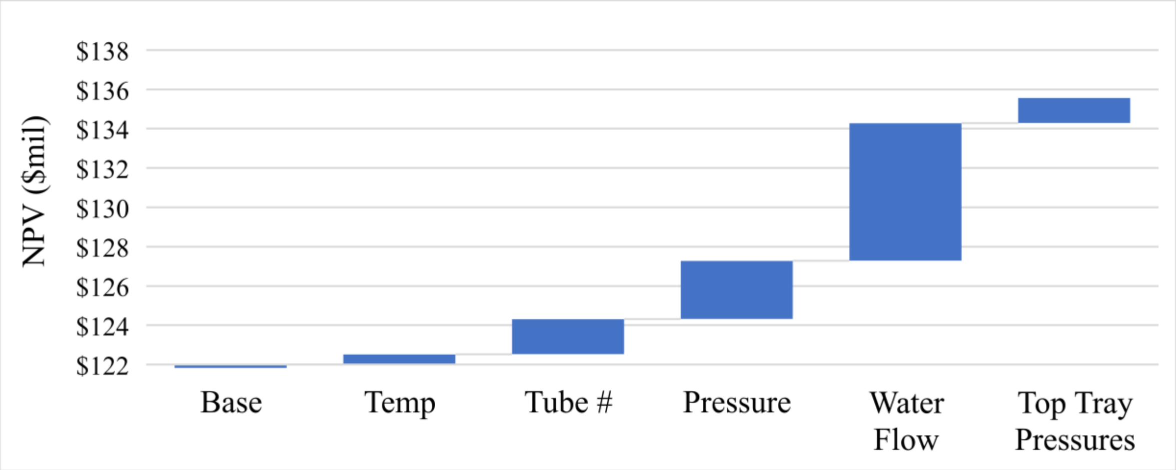

Figure 1: Waterfall chart, detailing changes to NPV per variable

Sensitivity Analysis

Various sensitivities throughout this process include acetone sales price, raw material cost, equipment cost, utilities cost, and labor cost, as seen in Figure 2. While factors such as acetone sales price and labor cost were assumed to be relatively constant for the life of the plant, factors such as utilities and equipment cost were able to be optimized. Even though they were assumed to be constant, the process is most sensitive to the sales price and raw material cost. If the prices were to fluctuate, it would significantly affect the rate of return on the project. Since the raw materials have such a large impact on the NPV, reducing their use was a key priority. Additionally, limiting the waste of acetone was also key to increasing the NPV. To reduce the equipment cost, the reactor size was greatly reduced. To recover as much acetone as possible, the water flowrate rate was increased, however, that increases equipment costs along the recycle.

Due to the 99.9 wt% minimum specification, there is not a large amount of allowance in terms of product quality. It would be possible to decrease product quality and sell a nonpharmaceutical grade acetone product. If a lower specification were produced, the sales price would be less, which would affect the process much more than the decreased utility cost. Given an acetone purity of 99.9 wt% from the optimization of this plant, there cannot be many more changes made and still meet the specifications.

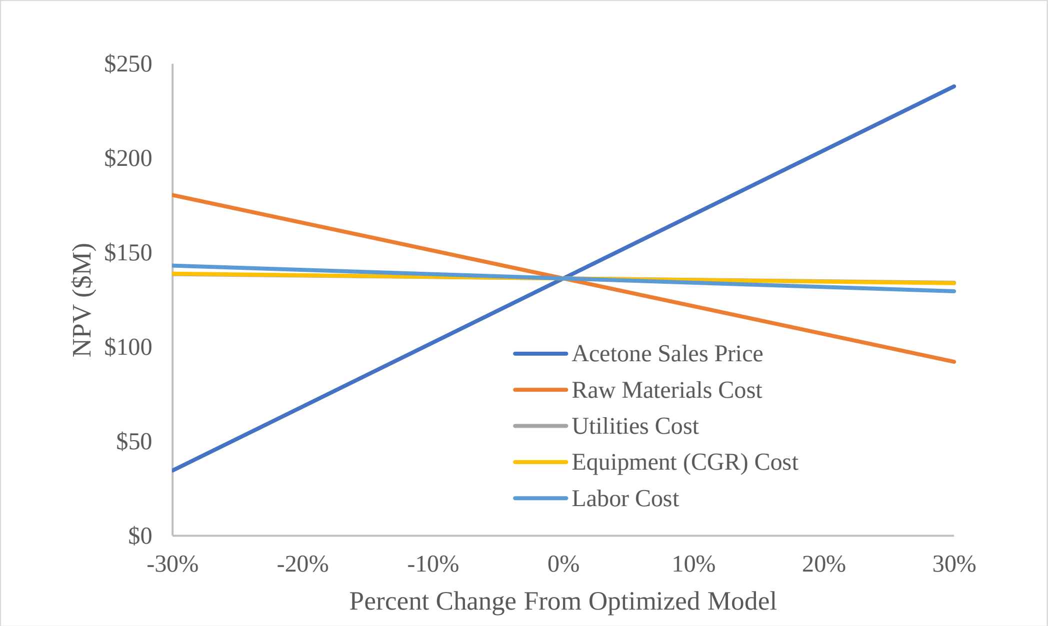

Figure 2: Sensitivity Chart

Optimization Logic

In the first round of optimization, three separate scenarios were considered: using the low temperature catalyst with high pressure steam as a heating medium, using the low temperature catalyst with NC17 as the heating medium, and using the high temperature catalyst with NC17 as the heating medium. In all three scenarios, the same variables were considered: reactor temperature, reactor volume, reactor pressure, and absorber water flowrate.

Using the high-pressure steam eliminated the need for the heater, which was the largest equipment contribution to the fixed capital investment (FCI). However, given the small temperature gradient between the 254°C steam and the 250°C reactor outlet stream, it was determined that the cost of the additional heat exchange area needed would be greater than the cost savings from eliminating the heater. In addition, the low temperature catalyst is required to be replaced every two years, while the high temperature catalyst is required to be replaced every three, ultimately increasing catalyst cost for the low temperature catalyst. The low temperature catalyst with high pressure steam produced an NPV of $110 million. The low temperature catalyst was investigated with NC17, which eliminates the need for the high heat exchange area, as a heater is utilized and can take on a higher duty for a lower reactor heat exchange area. However, given a large recycle due to a lower single-pass conversion inside the reactor, the NPV ultimately was $102 million for the low temperature catalyst with NC17 as a heating medium. After the first round of optimization, the high temperature catalyst had an NPV of $129 million. The process of the first and second rounds of optimization is detailed below for the high temperature catalyst using NC17 as a heating medium.

The first area selected to be optimized was the reactor conditions. The areas of temperature, pressure, and tube number were chosen. For temperature, it was elected to investigate a temperature increase. Increasing the temperature will increase the rate of reaction, therefore increasing the conversion to acetone due to the reaction kinetics (Turton, 2018). This can be seen through the increase of conversion from 88.4% at 350°C to 96.5% at 460°C. While the temperature increase continues to increase the conversion, the NPV begins to plateau at 460°C, and then further increases in temperature result in NPV decreases. The conversion becomes so high, that any further increase in temperature does not produce a significant increase in conversion. Also, the heater duty to maintain the reactor temperature becomes larger, resulting in more utility use. In the first round of optimization a temperature increase from the base case of

350 to 430°C was explored, and in the second round, a temperature range of 440 to 600°C was explored. Round 1 is shown in Figure 3 and round 2 is shown in Figure 4.

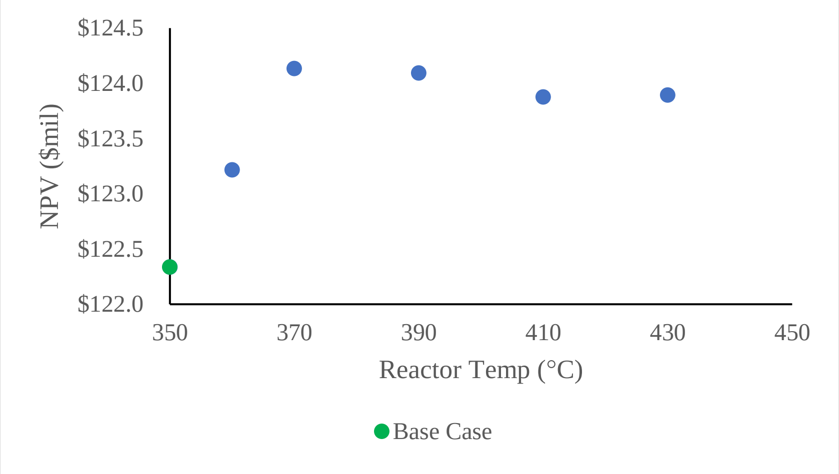

Figure 3: First Round of Optimization, Reactor Temperature - High Temperature Catalyst

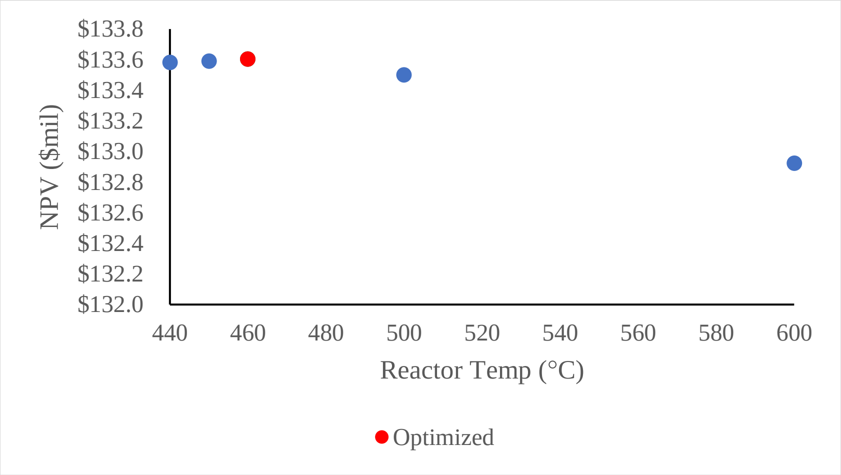

Figure 4: Second Round of Optimization, Reactor Temperature - High Temperature Catalyst

Due to the plateau in NPV, as well as concerns about the maximum temperature for the carbon steel reactor at 550°C, it is recommended to operate the reactor at 460°C.

The second area optimized was the reactor volume. This was achieved by varying the number of tubes in the reactor rather than other factors such as length to ensure the correct pressure drop was maintained throughout the reactor. While it would be expected that an increase in reactor volume would increase the conversion, and therefore increase the NPV, increasing the reactor volume increases the cost due to the additional catalyst. The reactor volume was explored in both the first and second round of optimization. The first round consisted of decreasing the base-case model from 450 to 390 tubes. After the trend showed an increase in NPV with fewer tubes, the second round explored 310 to 180 tubes. This is shown below in Figures 5 and 6. The base case value is highlighted in red.

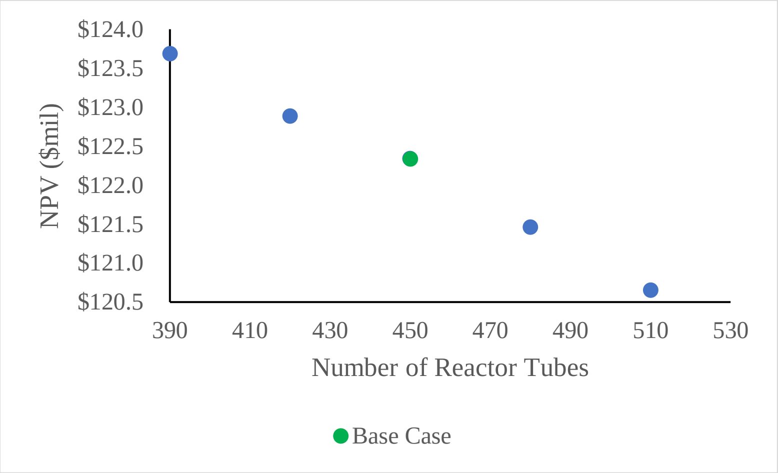

Figure 5: First Round of Optimization, Reactor Volume - High Temperature Catalyst

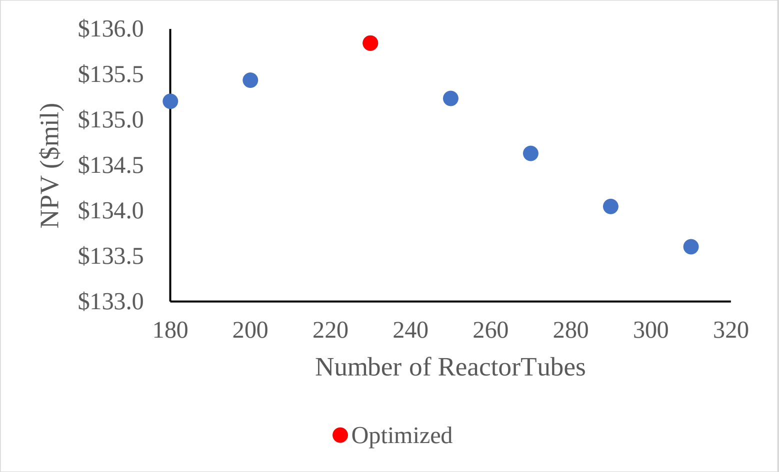

Figure 6: Second Round of Optimization, Reactor Volume - High Temperature Catalyst

During the first round of optimization, there was a clear trend showing that the reaction could proceed with fewer tubes without sacrificing conversion. However, the NPV no longer increases after 230 tubes, showing that the decrease in conversion from reducing tube number outweighs the savings from reducing the reactor volume. Due to the sharp peak at 230 tubes in the second round of optimization, it was determined that 230 tubes gave the optimal reactor volume.

The third area optimized was the reactor pressure. Given that this is a gas phase reaction, increased pressure will increase the partial pressure of the components, which increases the rate of reaction and the conversion, and therefore the NPV. However, given the stoichiometry of the reaction, increasing pressure could lead to the reaction shifting to the reactant side, as there are fewer moles on the reactants side compared to the products side (Turton, 2018). This will decrease the NPV due to the reaction shifting away from the acetone side. This was explored in both cycles of optimization, as shown below in Figures 7 and 8.

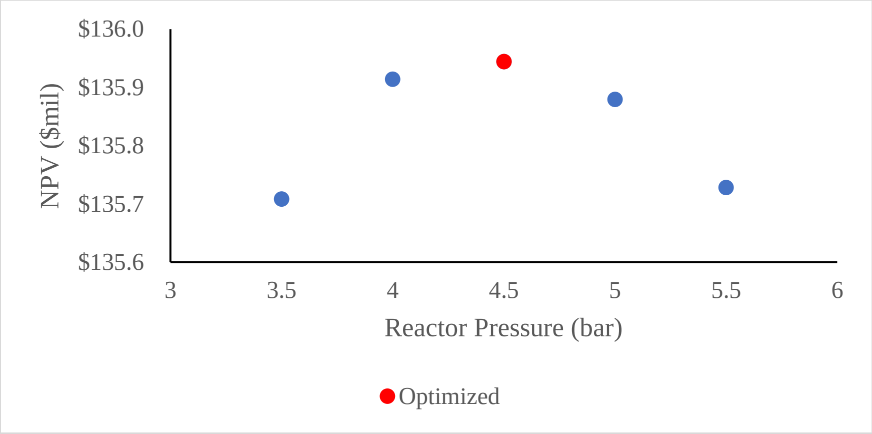

Figure 7: First Round of Optimization, Reactor Pressure - High Temperature Catalyst

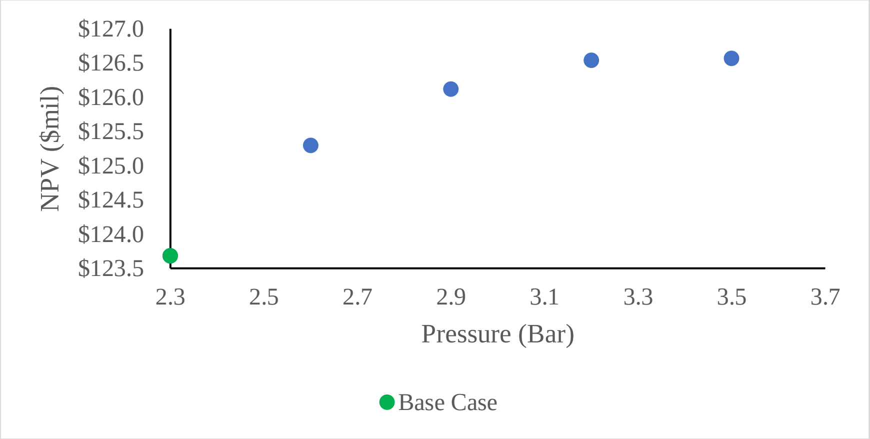

Figure 8: Second Round of Optimization, Reactor Pressure - High Temperature Catalyst

From the first round of optimization, it can be observed that an increase in pressure correlates to an increase in NPV, showing the positive effect pressure has on the gas concentrations. However, in the second round, it shows that after 4.5 bar the reaction stoichiometry begins to limit the positive effects of pressure. After 4.5 bar, the negative effects of pressure on stoichiometry cause the NPV to show a negative trend with increased pressure. The pressure containing the highest NPV is 4.5 bar, and therefore it is recommended to operate the reactor at this pressure.

The water flowrate to the absorber was also investigated in both rounds of optimization. For the absorber to separate the hydrogen from the organics, water is used as the absorbing fluid. Increasing the water allows better separation and will allow more acetone to be recovered. From Figure 1, the greatest gain in NPV occurred when the water flowrate increased. However, since both the water and acetone leave the absorber through the bottom, if water flowrate is increased too high, this can cause a dilution of the acetone product stream, causing the acetone to fail the 99.9 wt% minimum specification. To combat this, as water flowrate was increased, the first distillation tower specification was increased from 97% water recovery to the bottoms to 99% water recovery to the bottoms. This ensured there was less water able to exit through the acetone product stream. In addition, the condenser on this distillation tower was lowered from operating at 50°C to operating at 30°C to condense more water that would previously be sent through the acetone product stream. Since the minimum temperature of cooling water is 30°C, it could no longer be used as the cooling medium for the condenser. Therefore, refrigerated water had to be used. Implementing both strategies allowed the water flowrate to be increased from the base case of 41.5 kmol/hr to 61.5 kmol/hr in the first round of optimization and increased again in the second round from 61.5 kmol/hr to 161 kmol/hr. This can be seen in Figures 9 and 10.

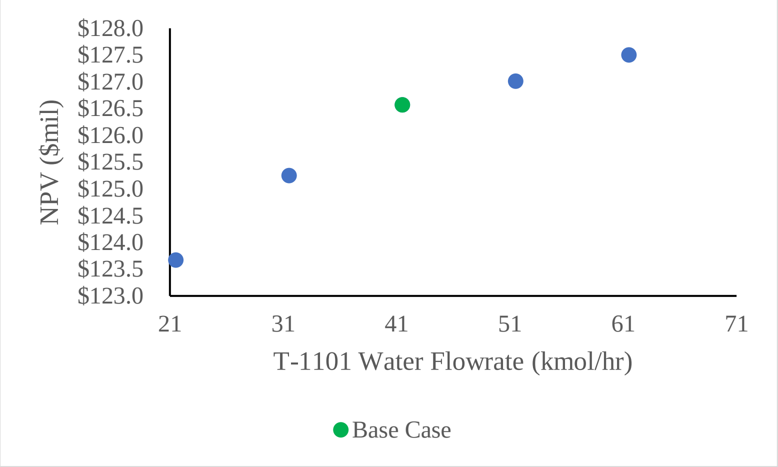

Figure 9: First Round of Optimization, Absorber Water Flowrate - High Temperature Catalyst

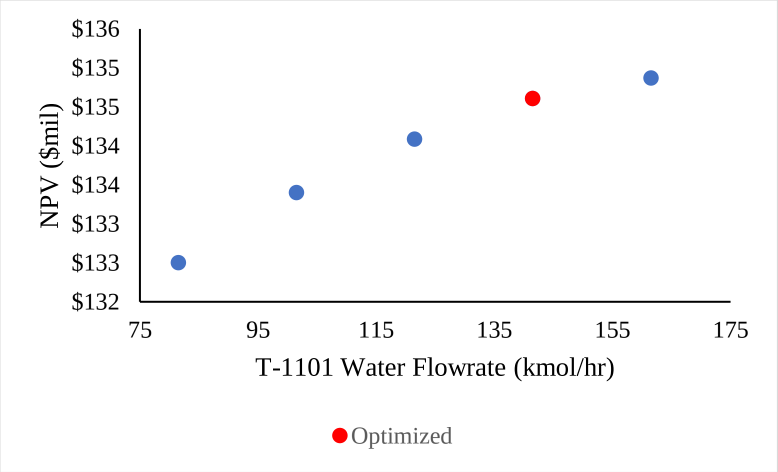

Figure 10: Second Round of Optimization, Absorber Water Flowrate - High Temperature Catalyst

In both the first and second rounds of optimization, an increase in absorber water flowrate resulted in an increased NPV. However, although this shows the NPV is greatest at 161 kmol/hr, it does not meet the minimum acetone product weight percent specification, so 153 kmol/hr is recommended as the operable water flowrate. This is the highest water flowrate that still meets the minimum weight percent specification of acetone.

Heat integration was explored to save on utility costs. The outlet of the reactor was used to heat the inlet to the reactor. This would save on both high-pressure steam and cooling water used to bring the streams to the desired temperatures. There are some downfalls to take into consideration with this layout. First, there is an increased risk of fouling on the shell side. Having a mixed heating medium with alcohol, water, hydrogen, and acetone could present challenges in the future. Clean steam would decrease the likelihood of fouling. Second, if there is a leak in a tube, contamination of the shell and tube sides could cause a premature reaction, affecting equilibrium in the reactor. Third, it may be difficult to control this process. If the outlet temperature of the reactor changes, it would change the inlet temperature as well. This causes a shift in equilibrium of the reaction. Due to the high purity specifications of the process, this would not be ideal for the separation section if there is a change in effluent composition. With all this in mind, it is not recommended to pursue heat integration. The small savings on utilities over the life of the project would not be worth the expenses from the extra maintenance and controls. While heat integration is not recommended, an expert should be consulted regarding the size of the heat exchangers and the temperature difference out of the tubes. It is suggested that tubes can only withstand a temperature difference up to 110°C. Adding a different heat exchanger configuration (2-4 or 3-6) could alleviate this problem (Turton, 2018).

Other factors that were explored but not implemented included tower sequencing and top tray pressure variation on both distillation towers. Currently, the towers are sequenced to separate the acetone product from the IPA before separating the IPA recycle from the wastewater. While the current process is sufficient, another method can be explored to achieve the required separation. The towers could be sequenced to remove the wastewater from the organic in the first distillation tower, and the acetone product could be removed from the IPA recycle in the second tower. Since the heat of vaporization for IPA and water are larger than acetone, it could be beneficial to separate the two first (Turton, 2018). A larger heat of vaporization will result in more duty being needed to complete the separation. If more duty is used for the first tower, the second tower will need less duty to complete the separation of the acetone product and the IPA. This process was simulated, and the duty on the reboiler and condenser on the first tower were decreased. Because there were less specifications needed for the first distillation tower, the condenser and reboiler did not need to supply as much energy as in the current case. Despite needing less duty in the first column, the second tower could not achieve a 99.9 wt% acetone. Also, this system costs about one million dollars more than the current model over the lifetime of the project due to a larger recycle stream. Therefore, it is not recommended to continue with this method. In addition, in varying the top tray pressure for both towers, minimal NPV increases were seen. Ultimately, the NPV for the high temperature catalyst was $136 million.

Process Safety and Environmental Considerations

Process safety was a crucial factor in the optimization process and played a key role in the decision-making process. With the reactor being made of carbon steel rather than a more temperature resistant material, the optimized reactor temperature was limited to 460 °C to prevent overheating of the reactor. Additionally, it is recommended that temperature alarms be added to the reactor with high and high-high alarms being added to the control system. These alarms will notify the operator to lower the NC-17 flowrate and lower the fuel gas to heater. Pressure relief valves should also be added to the reactor, distillation towers, and pressure vessels throughout the process to prevent damage due to over pressure situations. Two relief valves should be used rather than a single relief valve. A single relief valve has a failure rate of 1/100 so by adding two valves, this decreases the failure rate to 1/10,000. Burst discs can be added upstream of the relief valves to prevent any process fluids from contacting the pressure relief valves (Gill, 2023). This may not be necessary as acetone and IPA are not particularly susceptible to fouling, however it prevents these chemicals from damaging flange seals and polymer components of the valves. With acetone and IPA having flash points -17.8 °C and 12.2 °C respectively, the process streams will contain potentially flammable atmospheres. To mitigate this hazard, it is recommended that flame arrestors be added to process streams to prevent explosion hazards from downstream equipment and igniting other areas of the plant. To supplement this, oxygen (O_2) analyzers will be added to flammable process streams to detect elevated levels of O_2 in streams. By monitoring O_2 levels, flammable atmospheres will be easily detected and indicate that there are issues in the process causing air to infiltrate into the system. Insulation should be applied to all hot surfaces on equipment unless it causes issues with overheating. There should be a valve on the fuel gas stream coming out of the absorber. This stream combines with the vapor stream flowing out of the flash drum on the first distillation tower, which is at 1.2 bar. It is important to reduce the pressure of the fuel gas stream to prevent backflow into the flash drum; there could be a pressure build up in the drum, causing safety hazards to personnel and equipment.

Global, Cultural, Social, and Economic Factors

The global markets for acetone, IPA, and acetone consuming industries are of key importance when determining the future economic outlook for this facility. Acetone is used in the production of many chemicals such as Bisphenol A (BPA), solvents, oils, rubbers, and resins. With acetone being used in such a wide variety of industries, this diversified list of acetone consumers lowers the impact that market variations could have on acetone, thus making a safer economic investment in this facility. With the compound annual growth rate for acetone, IPA, and BPA ranging 6-8%, there is considerable growth for the acetone industry in the future (Grandview, 2023). Location is also an important factor for the construction of chemical plants. If this plant is built along the Mississippi River, this would allow product shipment by boat and travel to other areas of the U.S. The acetone demand is growing more rapidly in European markets compared to North America, and the access to the Gulf of Mexico would allow for trade in these international markets.

Although profitability is the cornerstone of this optimization, there are many factors which are important to consider when discussing this acetone production facility. For example, this facility will require 12 operator positions and an engineering, a maintenance, and an administrative staff. This will increase employment in the surrounding community and help provide stable jobs. The presence of this facility could also attract other companies to the area such as contractors, acetone consumers, etc. Factoring in the yearly income taxes and the taxes due to depreciation of equipment, the unit will be contributing roughly $11 million back into the community through state and local taxes. This tax money will go towards useful public programs such as education, road maintenance, public parks, and emergency services.

Report Recommendation

It is recommended that the company pursue a more in-depth economic analysis of this project. As seen from the optimization, there is a significant return on investment for the project. Additionally, the acetone can be made in a safe and environmentally friendly manner. The optimized design should undergo a more detailed process of optimization by simultaneously changing the variables. This will push closer to a true optimum for the process. The engineers on this team are seeking endorsement to begin work on these next steps.

Additional Optimization: Fluidized Bed Reactor

Fluidized bed reactors are used in the chemical industry to turn raw material into products. They are often applied to gas phase reactions. These reactors can be prone to erosion due to fast moving particles. Also, bubbles forming within the reactor cause fluid to bypass the catalyst, resulting in a lower single-pass conversion. Despite these disadvantages, fluidized beds offer better heat transfer and the ability to transport process materials with a wide range of size distribution. Therefore, fluidized bed reactors are best used in processes requiring the use of a catalyst and superior heat transfer (Wen, 1966).

Due to these advantages, an isothermal fluidized bed reactor will be utilized to dehydrogenate IPA into acetone and hydrogen. The objective of this optimization is to optimize the selectivity and conversion of acetone to IPA in the effluent by altering the inlet pressure, inlet temperature, volume, and length to diameter (L/D) ratio of the reactor in a linear fashion. The selectivity is the ratio of desired product, acetone, to the ratio of undesired product, IPA. There are multiple constraints that will need to be considered while optimizing the reactor. First, the operating temperature of the reactor needs to be within the temperature range of the catalyst. Second, due to the bubbling nature of the fluid, about 10% of the feed gas bypasses the catalyst. Therefore, the single-pass conversion can never exceed 90%. Third, the length of the reactor must be larger than 6.1 m to fit the heat exchange tubes. Finally, the ratio of the superficial gas velocity to the minimum fluidizing velocity (μ_{mf}) needs to be in the range of 3 – 10. The value of μ_{mf} can be calculated using the Wen and Yu correlation in equation 2 below:

$$Re_{p,mf} = \frac{\mu_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408Ar]^{0.5} - 33.7 \qquad \text{(Eqn. 2)}$$

where *Ar* is the Archimedes number in equation 3,

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

d_p, the particle diameter; ρ_g, the gas density; μ_g, the gas viscosity; ρ_s, the catalyst density; and g, the acceleration due to gravity (Wen, 1966).

A simulation was designed to represent the reactor. The reactor was initially set to 8 m long and 2 m in diameter, which yields a volume of 25.13 m^3. The feed into the reactor was maintained constant at 100 kmol/hr to mimic the flowrate into R-1101 in Unit 1100. An initial temperature of 300°C and a pressure of 0.75 bar were set to get a base case for the reactor. The selectivity at these operating conditions was 0.116.

Because of the reactor's sensitivity to pressure drop, pressure was the first variable optimized. Pressures in the range of 0.75 to 5 bar were observed. The optimum pressure for the reactor at 300°C and 25.13 m was found to be 1.125 bar, which yielded a selectivity of 2.50. Figure 11 reflects the optimum pressure of 1.125 bar shown in red.

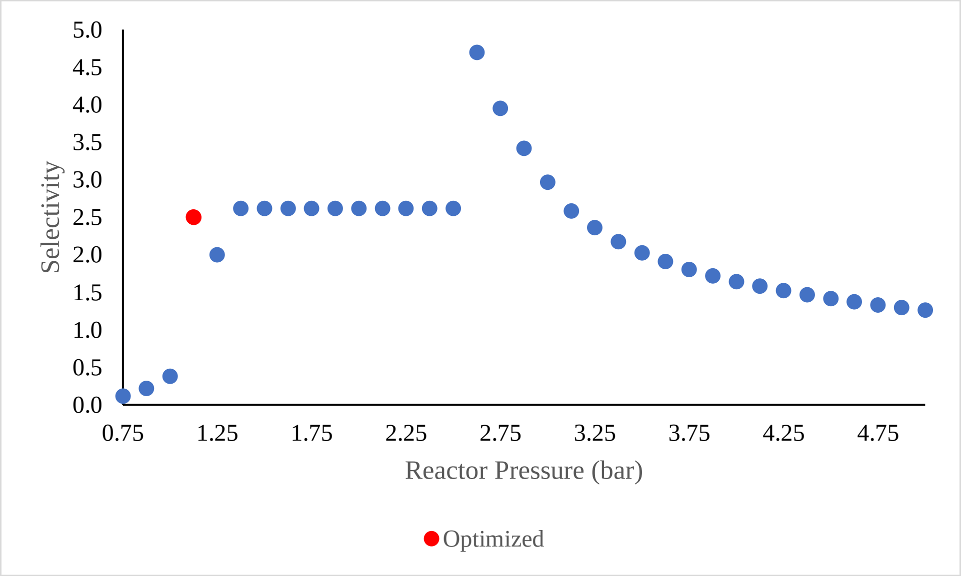

Figure 11: Selectivity vs Reactor Pressure Graph

While pressures 2.6 through 3.125 bar had a larger selectivity, the velocity ratios of the inlet and outlet did not fall into the constraint. Additionally, pressures 1.375 to 2.5 bar would not converge due to the volumetric flowrate being too large. As the pressure increased, there was more conversion in the reactor, causing more hydrogen and acetone to be produced. Since hydrogen and acetone take up more volume than the IPA, there will be a larger pressure drop through the reactor. Since this pressure drop is too large, the reactor at the current dimensions could not handle the conversion. As pressure increases, the reaction will favor acetone formation because of the increase in concentration. The kinetics of the reaction are dependent on the concentration, so when the concentration increases, the conversion will increase. However, once the pressure reaches a certain level, the reaction will start to favor the formation of IPA. Thermodynamically, as the pressure increases, a reaction will shift to the side with the least moles. Since the reactants side has one mole (IPA), and the products side has two moles (acetone and hydrogen), more IPA will be formed (Turton, 2018).

The next variable altered was inlet temperature. Temperatures in the range of 300°C and 700°C were observed. A temperature of 310°C was chosen as the optimum for the given application, which yielded a selectivity of 3.18. Figure 12 shows the temperatures, and the optimum temperature of 310°C is in red.

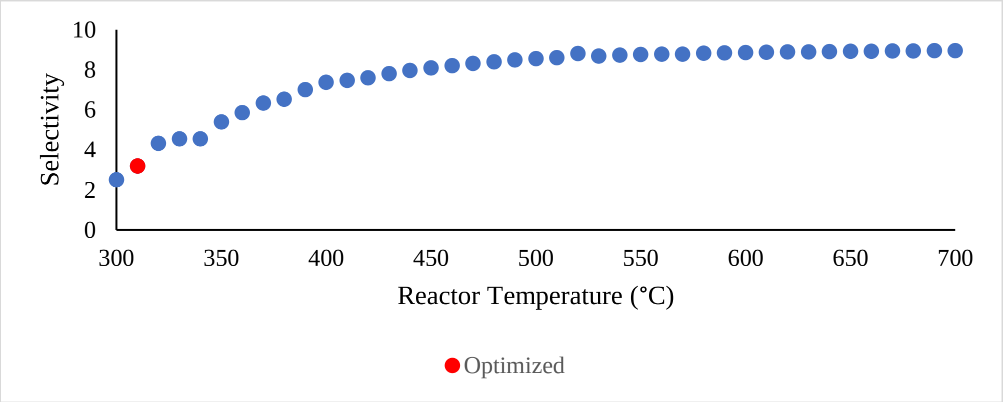

Figure 12: Selectivity vs Reactor Temperature Graph

As the temperature increased, the selectivity increased. When the temperature increases, the kinetics of the reaction favors the formation of acetone. However, as the temperature increases, the volumetric flowrate of the inlet and outlet also increases. Hence, the velocity ratio does not fit into the given constraints (Turton, 2018).

After temperature, the volume of the reactor was evaluated. Volume was changed by varying the length of the reactor and calculating a diameter that satisfied a L/D ratio of 4. A volume of 40.77 m^3 was chosen as the optimum for the given application, which yielded a selectivity of 3.89. Figure 13 shows the volumes of the reactor, and the optimum volume of 40.77 m^3 is in red.

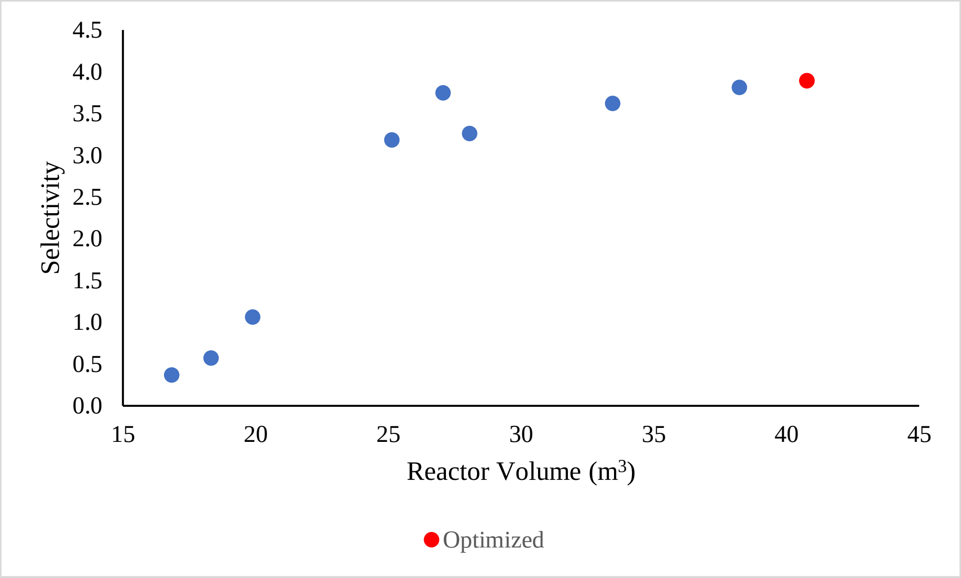

Figure 13: Selectivity vs Reactor Volume Graph

As the volume increases, the conversion will also increase. Therefore, selectivity will also increase (Turton, 2018). The volume chosen was 40.77 m^3.

The final variable changed was the L/D ratio. The optimum L/D ratio for the previous variables was 4, which kept the same selectivity of 3.89. Figure 14 shows the L/D ratios, and the optimum L/D ratio of 4 is in red.

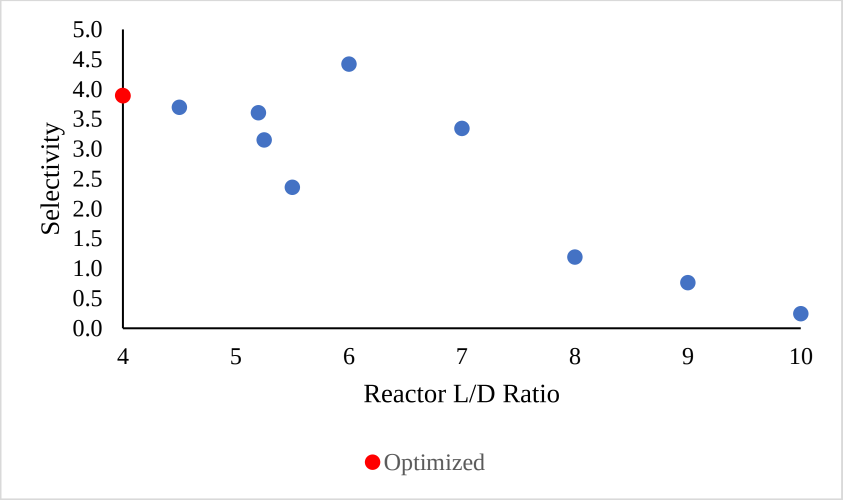

Figure 14: Selectivity vs Reactor L/D Ratio Graph

Increasing the L/D ratio will decrease the diameter. As the diameter decreases, the flowrate of the vapor will increase, causing a decrease in residence time. The decrease in residence time will cause the conversion in the reactor to decrease. While the L/D ratio of 6 had the largest selectivity, the velocity ratio did not meet the specifications. L/D ratios between 2 and 4 did not converge because of pressure drop considerations (Turton, 2018).

After the 4 optimizations, the optimal reactor operating conditions were an inlet temperature of 310°C, an inlet pressure of 1.125 bar, a volume of 40.77 m^3, and a L/D ratio of 4. This configuration gives a selectivity of 3.89. This reactor should be examined in the future for pricing considerations and further optimization.

Bibliography

Acetone market size, share, Trends & Growth Report, 2030. Acetone Market Size, Share, Trends & Growth Report, 2030. (n.d.). Retrieved April 27, 2023, from https://www.grandviewresearch.com/industry-analysis/acetone-market

Turton, R. (2018). *Analysis, synthesis, and Design of Chemical Processes*. Prentice Hall.

Harrelson, J., Smith, A., & Gill, M. (2023). *Production of Acetone*. Lecture, Oxford, MS.

Gill, M. (2023). *Ch E 452: Process Safety*. Lecture, Oxford, MS.

Wen, C.Y., and Y.H. Yu (1966). *AIChE J.,* 12, 610.

APPENDICES

Appendix A: Process Flow Diagram for Base Case and Optimized Design

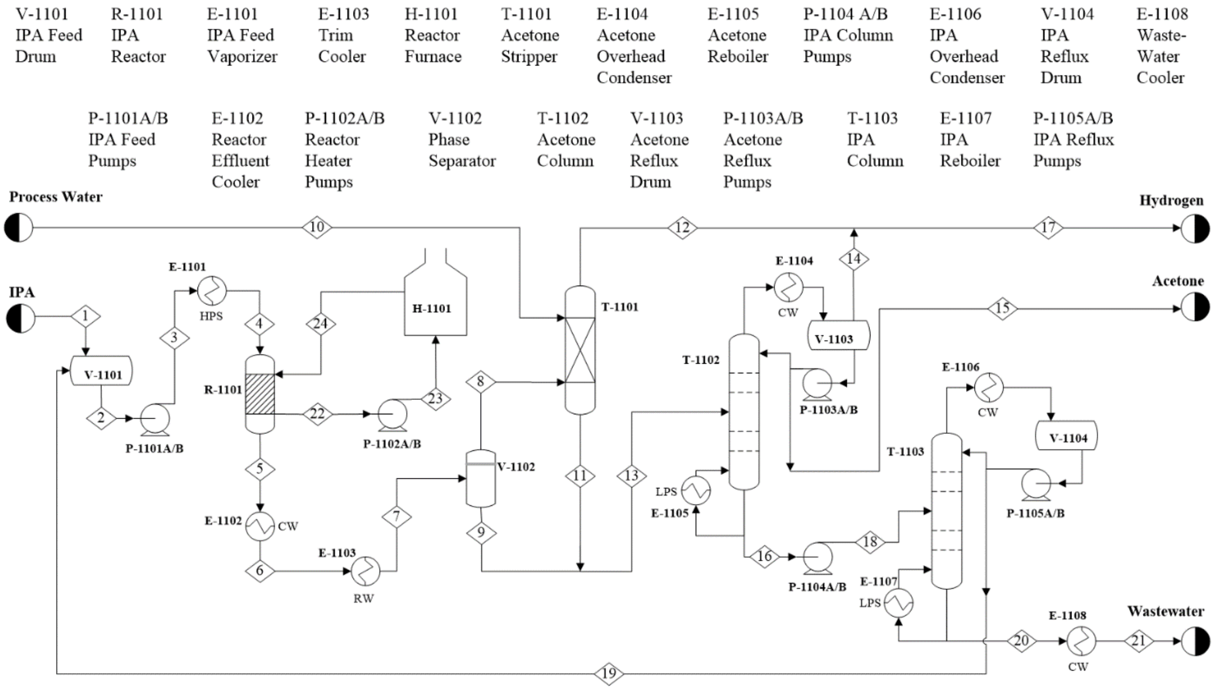

Figure A-1: Process Flow Diagram for Base Case and Optimized Design

Appendix B: Base Case Stream Table

Table B-1: Base Case Stream Table

Stream No.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Temperature (°C)	25.0	32.6	32.6	240.0	350.0	45.0	20.0	20.0	20.0	25.0	26.3	34.8
Pressure (bar)	1.0	1.0	2.3	2.2	2.0	1.9	1.7	1.7	1.7	2.0	1.6	1.5
Vapor Mole Fraction	0.0	0.0	0.0	1.0	1.0	0.5	0.4	1.0	0.0	0.0	0.0	1.0
Total Mass Flow (MT/h)	4.8	5.5	5.5	5.5	5.5	5.5	5.5	0.6	4.8	0.7	0.9	0.4
Total Molar Flow Rate (kmol/h)	104.4	118.5	118.5	118.5	188.5	188.5	188.5	78.4	110.1	41.5	43.4	76.5
Component Flowrate (kmol/hr)												
Hydrogen	0.0	0.0	0.0	0.0	69.9	69.9	69.9	69.5	0.4	0.0	0.1	69.4
Acetone	0.0	0.3	0.3	0.3	70.2	70.2	70.2	7.9	62.3	0.0	3.5	4.4
IPA (Isopropyl Alcohol)	69.9	79.1	79.1	79.1	9.1	9.1	9.1	0.2	8.9	0.0	0.2	0.0
Water	34.4	39.2	39.2	39.2	39.2	39.2	39.2	0.8	38.4	41.5	39.5	2.8
NC-17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Stream No.	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Temperature (°C)	21.4	50.0	50.0	91.4	35.5	91.4	83.3	109.2	45.0	360.0	360.0	402.7
Pressure (bar)	1.6	1.2	1.5	1.4	1.2	1.5	1.2	1.4	1.3	30.0	30.5	30.3
Vapor Mole Fraction	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Mass Flow (MT/h)	5.8	0.1	3.7	2.0	0.5	2.0	0.7	1.3	1.3	36.1	36.1	36.1
Total Molar Flow Rate (kmol/h)	153.4	1.5	64.8	87.1	78.0	87.1	14.2	73.0	73.0	150.0	150.0	150.0
Component Flowrate (kmol/hr)												
Hydrogen	0.5	0.5	0.1	0.0	69.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Acetone	65.8	1.0	64.5	0.3	5.4	0.3	0.3	0.0	0.0	0.0	0.0	0.0
IPA (Isopropyl Alcohol)	9.1	0.0	0.0	9.1	0.0	9.1	9.1	0.0	0.0	0.0	0.0	0.0
Water	77.9	0.0	0.2	77.7	2.8	77.7	4.7	72.9	72.9	0.0	0.0	0.0
NC-17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	150.0	150.0	150.0

Appendix C: Optimized Stream Table

Table C-1: Optimized Stream Table

Stream No.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Temperature (°C)	25.0	28.3	28.5	240.0	460.0	45.0	20.0	20.0	20.0	25.0	27.9	26.5
Pressure (bar)	1.0	1.0	4.5	4.4	4.1	3.9	3.8	3.8	3.8	2.0	1.6	1.5
Vapor Mole Fraction	0.0	0.0	0.0	1.0	1.0	0.4	0.4	1.0	0.0	0.0	0.0	1.0
Total Mass Flow (MT/h)	4.5	4.7	4.7	4.7	4.7	4.7	4.7	0.3	4.4	2.8	2.9	0.2
Total Molar Flow Rate (kmol/h)	104.4	118.5	118.5	118.5	188.5	188.5	188.5	78.4	110.1	41.5	43.4	76.5
Component Flowrate (kmol/hr)												
Hydrogen	0.0	0.0	0.0	0.0	65.3	65.3	65.3	64.4	0.9	0.0	0.4	64.0
Acetone	0.0	0.3	0.3	0.3	65.6	65.6	65.6	3.3	62.3	0.0	3.1	0.3
IPA (Isopropyl Alcohol)	65.4	67.7	67.7	67.7	2.4	2.4	2.4	0.0	2.3	0.0	0.0	0.0
Water	32.2	36.6	36.6	36.6	36.6	36.6	36.6	0.3	36.3	153.0	151.8	1.5
NC-17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Stream No.	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**
Temperature (°C)	24.0	30.0	30.0	102.6	26.7	102.6	82.2	109.2	45.0	360.0	360.0	406.3
Pressure (bar)	1.6	1.2	1.5	1.4	1.2	1.5	1.2	1.4	1.3	30.0	30.5	30.3
Vapor Mole Fraction	0.0	1.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Mass Flow (MT/h)	7.3	0.0	3.8	3.5	0.2	3.5	0.2	3.3	3.3	0.0	0.0	0.0
Total Molar Flow Rate (kmol/h)	153.4	154.4	155.4	156.4	157.4	158.4	159.4	160.4	161.4	162.4	163.4	164.4
Component Flowrate (kmol/hr)												
Hydrogen	1.3	1.2	0.1	0.0	65.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Acetone	65.4	0.5	64.5	0.3	0.8	0.3	0.3	0.0	0.0	0.0	0.0	0.0
IPA (Isopropyl Alcohol)	2.4	0.0	0.0	2.4	0.0	2.4	2.3	0.1	0.1	0.0	0.0	0.0
Water	188.1	0.0	0.2	187.9	1.5	187.9	4.4	183.5	183.5	0.0	0.0	0.0
NC-17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	150.0	150.0	150.0

Appendix D: Optimized Utility Table

Table D-1: Optimized Utility Table

Exchanger ID	**E-1101**	**E-1102**	**E-1103**	**E-1104**	**E-1105**	**E-1106**	**E-1107**	**E-1108**
In	hps	cw	rw	rw	lps	cw	lps	cw
Out	bfw	cw ret	rw ret	rw ret	bfw	cw ret	bfw	cw ret
Temp (^oC)	234.00	350.00	45.00	30.00	92.00	108.80	108.80	108.80
Pressure (Barg)	1.30	0.91	0.77	0.63	0.63	0.50	0.50	0.40
Duty (GJ/h)	5.07	5.24	0.56	18.82	22.19	1.35	1.42	0.89
Price ($/GJ) IN	5.66	0.38	4.77	4.77	4.54	0.38	4.54	0.38
Price ($/GJ) OUT	1.52	0.38	4.77	4.77	1.52	0.38	1.52	0.38

Appendix E: Base Case Cash Flow Diagram

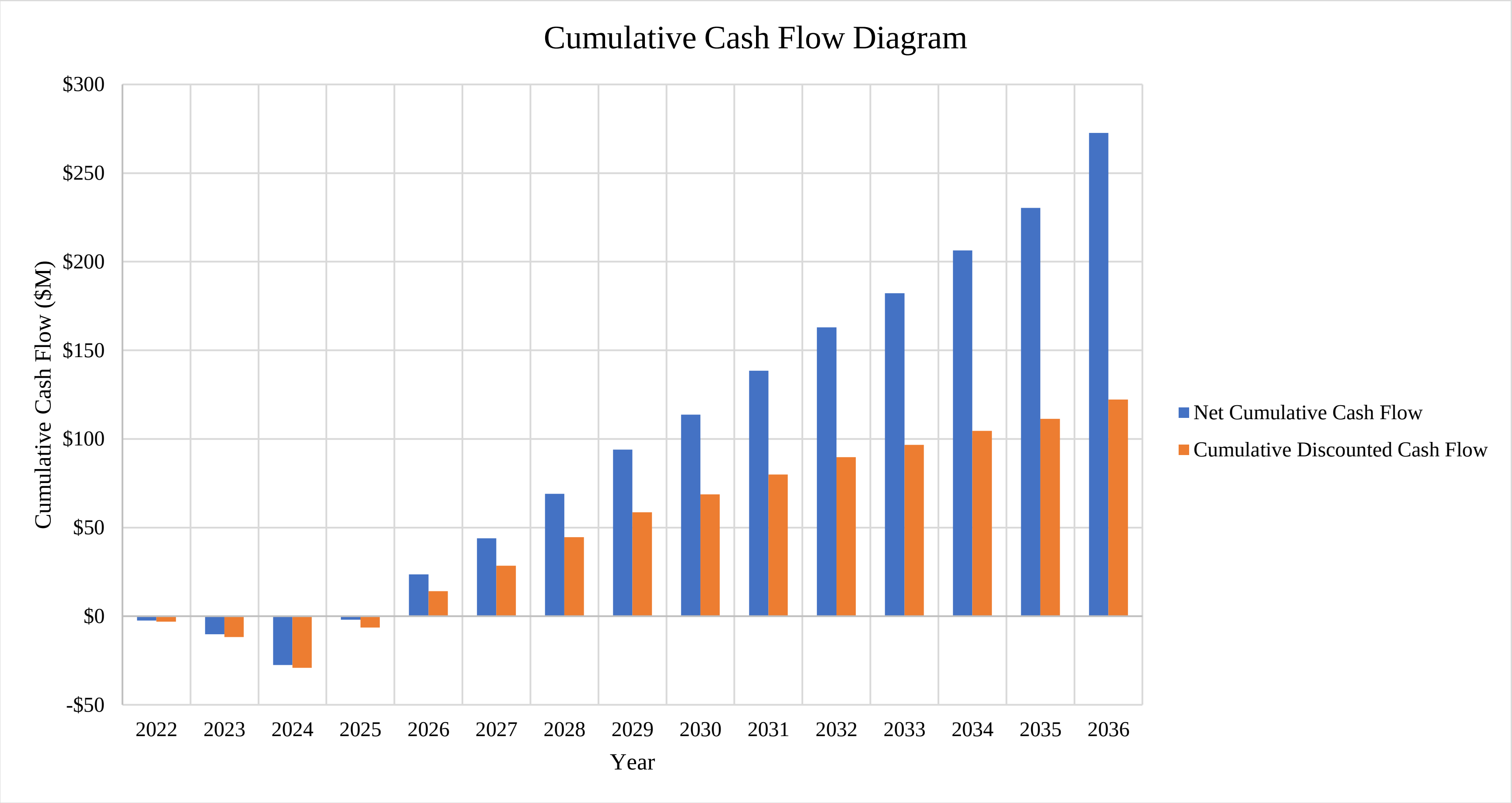

Figure E-1: Base Case Cash Flow Diagram

Appendix F: Optimized Cash Flow Diagram

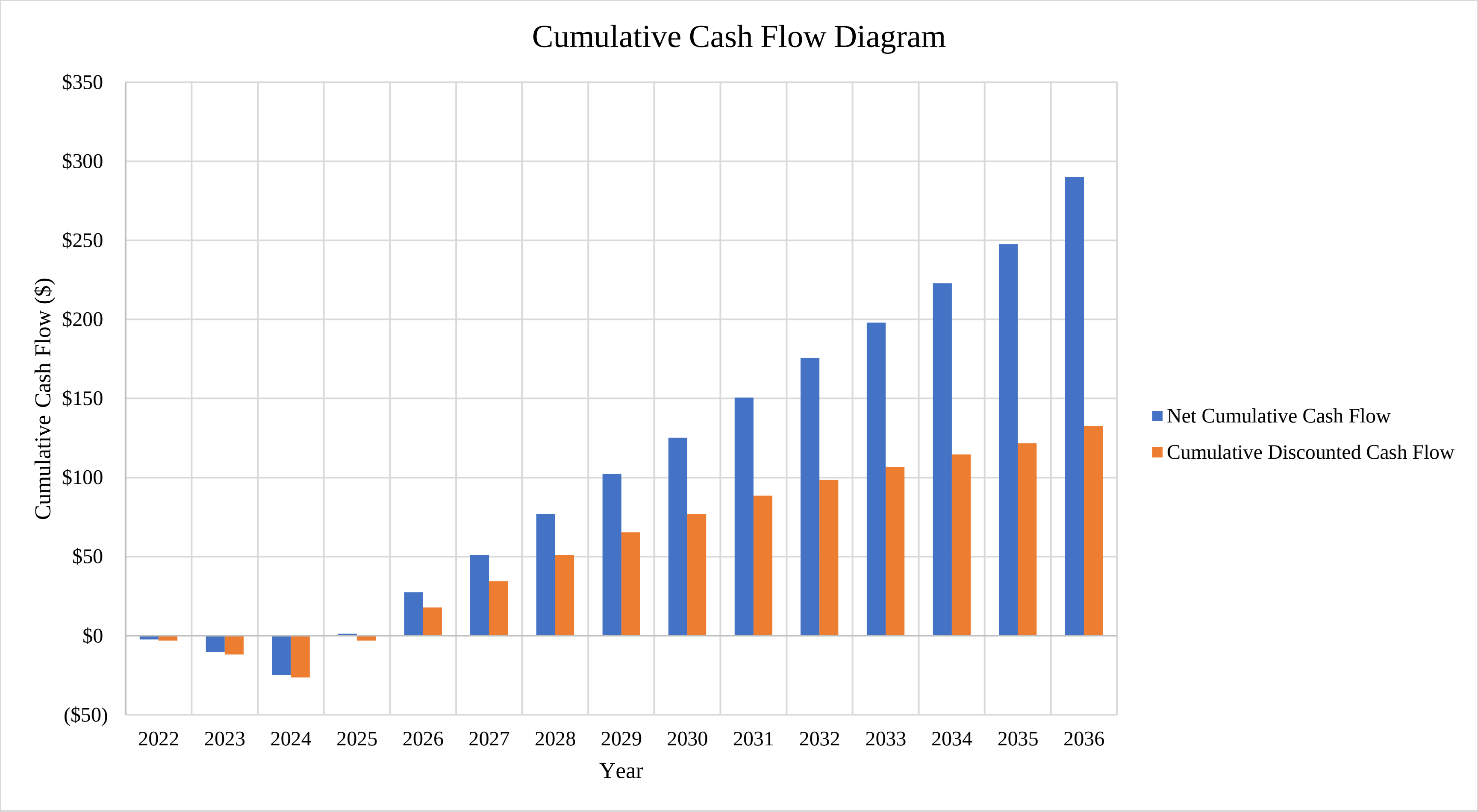

Figure F-1: Optimized Cash Flow Diagram