

Production of Acrylic Acid through the Oxidation of Propylene

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Group 27






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1 EXECUTIVE SUMMARY

This report aims to examine the synthesis of acrylic acid by propylene oxidation. Other methods of acrylic acid synthesis were investigated, but oxidation was selected based on a promising profit upper bound, easy separation, and lack of dependence on heavily fluctuating feedstock, biological hazards, and multiple expensive catalysts. The goal is to obtain a stream of 99.9% pure acrylic acid at a minimum of 50,000 tonnes/year and to purify byproduct acetic acid to 95% purity. The reactive part of the process combined gaseous propylene with oxygen then reacted in the presence of a catalyst. The oxygen is sourced from compressed air at 300kPa. Once the two are mixed, they are fed into a reactor of diameter 1.4 m and length 15 m with 20,000kg catalyst. The reactor is held at 250 °C and has a mean residence time of 81.6 seconds.

The material exiting the reactor is fed to a flash drum operating at 50 °C, which condenses the water, acrylic acid, and acetic acid. The gas stream has minimal acrylic acid, acetic acid, and propylene and is not worth recycling or separating. The liquid enters the first column in a two stages separation train. The first is a vacuum distillation column that separates acrylic acid into the bottoms while maintaining a low enough temperature as to not cause polymerization. The second column separates water from the bottoms of acetic acid. The process produces 51,900 tonne/year of 99.9% pure acrylic acid and 2,056 tonne/year of acetic acid from a side reaction that is purified to 95.3% purity, assuming 8,000 hours per year of operation. The entire process is a net positive energy, producing 3,230 kJ/h. In order to lessen energy costs, the cooling water being used on the reactor segments is pumped to the reboilers to help run both separation columns. This process requires an input of 33,199 tonne/year of propylene and 287,400 tonne/year of air. Upon exiting the separation train, the acrylic acid and acetic acid each feed into their own cone roof tank of 71,500 and 3000 gallons, respectively, which can each support 48 hours of production.

With a PUB between \$410-1,220 per tonne, the oxidation of propylene is a promising synthesis route. The simulation results suggest a profitable venture with almost \$168,233,745 million NPV and 99.76% IRR. The majority of the costs, \$34.5 million go to propylene feedstock. However, the flammability of propylene does pose a safety concern. It also has negative buoyancy and will form a cloud on the ground, which can lead to asphyxiation and is a fire risk. These factors mean that containment and proper industrial hygiene is of utmost importance. Waste propylene must be completely flared before exiting the factory, avoiding environmental release.

We recommend that further process exploration consider having a smaller reactor and recycling the unreacted propylene. This would reduce catalyst cost, which is a yearly investment, while still achieving complete reaction. Pure oxygen should also be considered to force more complete reaction in a significantly smaller area than when using air, as the cost saved in catalyst could offset the cost of oxygen.

2 INTRODUCTION

Acrylic acid ($C_3H_4O_2$) is an organic molecule that is valuable for its use in industry. Specifically, acrylic acid is synthesized for its use in ester synthesis, and is commonly found in the water treatment and textiles industry.¹ Multiple methods exist that can produce acrylic acid on an industrial scale; however, the most common and regularly used method is the oxidation of propylene. This method is used for the easily available reactants and ease of synthesis. Propylene is a byproduct of oil and natural gas refining and is under great demand across multiple industries, and is therefore produced in large quantities. This reaction process has considerably favorable yields for acrylic acid while producing acetic acid as a side product, which can also be of value when purified. There is also a favorable profit upper bound (PUB) of \$410-1,220 per tonne. However, this process does not lack drawbacks. From a safety perspective, propylene is a highly flammable substance (NFPA value of 4) that has a higher density than air, making leaks potentially deadly. From an economic perspective, this process is currently attractive, though the cost of raw natural gas and oil must be considered. Current prices for importing natural gas are \$1.63 per cubic foot and \$3.2 per cubic foot for industrial use by pipeline, which are record lows since the US Energy Information Administration began collecting data on each source.²

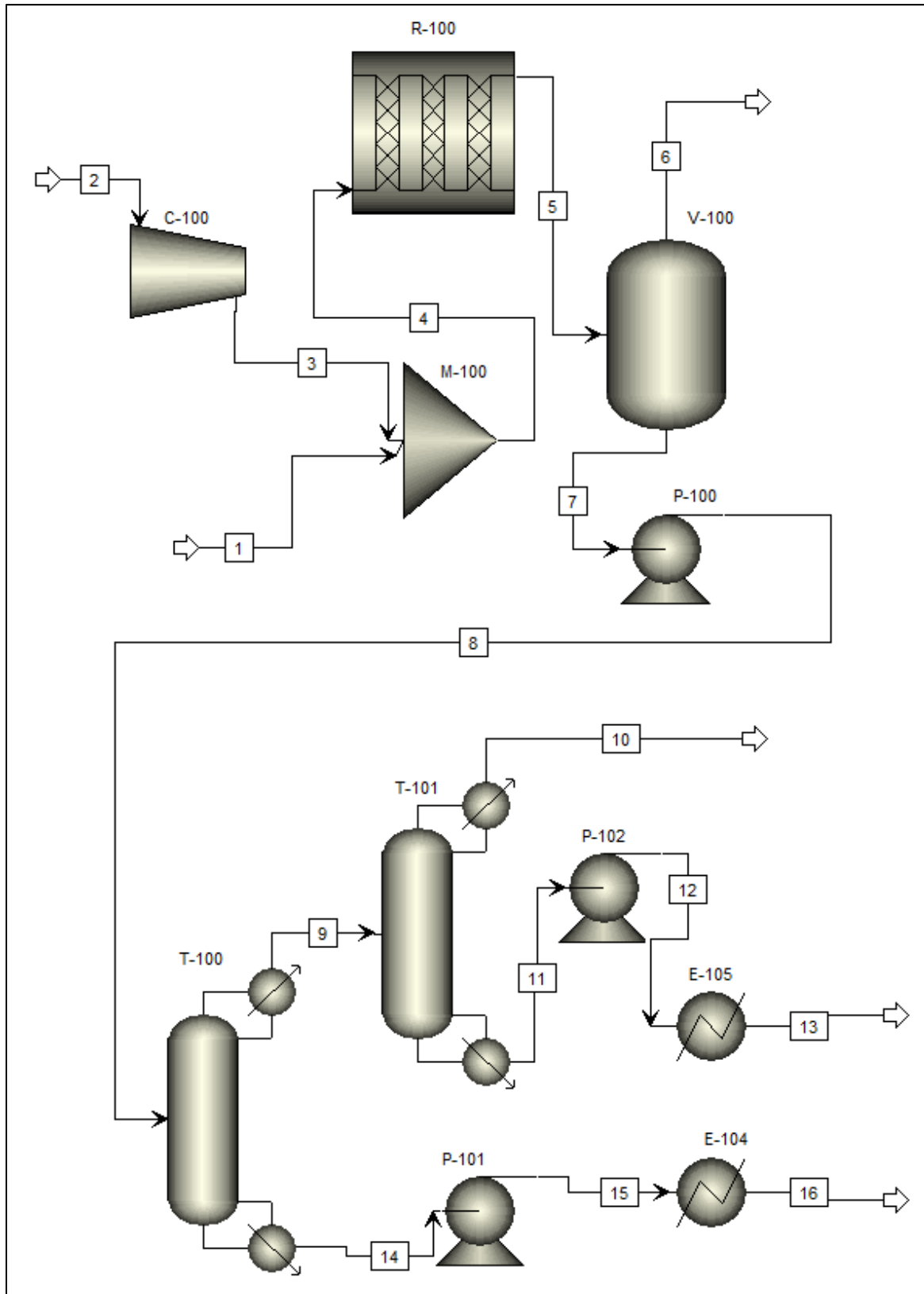
As stated before, oxidation of propylene is just one of many synthesis paths possible to produce acrylic acid. One such method is the fermentation of glucose. This process uses bioreactions to convert glucose to acrylic acid. The process starts as genetically modified *E. coli* converts the glucose in corn to 3-Hydroxypropionic acid (3-HP). 3-HP is produced via the malonyl-CoA pathway, which is converted from acetyl-CoA by the enzyme acetyl-CoA carboxylase. Cheng et al. constructed this pathway in *E. coli* by expressing the acetyl-CoA carboxylase from *Corynebacterium glutamicum*, and the malonyl-CoA reductase from *Chloroflexus aurantiacus*.⁵ 3-HP then undergoes dehydration to produce acrylic acid and water, which is purified by distillation. This method offers a more eco-friendly alternative, as the process offers significantly less carbon dioxide production and sources reactants from renewable carbon sources, such as corn. This process also offers commercial and dependency advantages, as a significant amount of corn suitable for this process is already grown in the United States. There would be significantly lower transportation costs for the domestic reactants, as well as a limited dependence on foreign oil and the fluctuating cost of fossil fuels. Finally, the process has the perk of producing almost exclusively water and acrylic acid, without major impurities or large amounts of waste. The downsides to this process include dependence on crop production and excess generation of wastewater. Such a substantial amount of corn poses to disrupt the corn market, possibly increasing the price of the currently inexpensive crop, as well as driving larger corn production, which could significantly threaten the water sources in the American Heartland. Safety must also be considered, as the process also requires usage of caustic and flammable organics and corrosive acids, as well as *E. coli*, which could pose major health risks to plant workers. The profit upper bound for this process ranges from \$-80 to 600 dollars per tonne. Because any negative market fluctuations, such as the price of corn going up, would lead to a steep drop in profits, and due to the upper end of the PUB being lower than other lower end of another process' PUB, this synthesis method was not chosen to be used.

A second alternative reaction route to form acrylic acid is the dehydration of glycerol. This is a two-step process in which glycerol is reacted in the presence of an acid (normally a Brønsted acid catalyst) to form acrolein. Acrolein is then subjected to molecular oxygen in the presence of a metal catalyst. This method had a promising profit upper bound of \$990-1642 per tonne. Other benefits include having very

little separation required, as only four products, acrylic acid, water, oxygen, and unreacted glycerol, which are decently easy to separate. The lack of a large amount of waste product and the lack of any hazardous or expensive-to-dispose-of product makes this reaction very attractive. It is also a benefit that glycerol is renewable and can be extracted from plant and animal sources or produced through a saponification reaction. These, coupled with the high PUB offer a tempting process to potential investors. However, a major downside to this reaction is that it requires two separate catalysts, one for each step of the reaction, that can be quite expensive, running anywhere from around a dollar per gram to a dollar per milligram.^{3,4} This will cut into profitability significantly. The second step of the reactor is particularly expensive to build, as it is a molybdenum or vanadium-based metal catalyst or a zeolite, both of which are susceptible to high levels of coking. Due to all these negative aspects, especially the expense of catalysts, the glycerol dehydration was not determined to be a good synthesis route to continue with.

The following report details a process with a goal to produce 50,000 tonnes of acrylic acid per year using the oxidation of propylene. The inputs, air and propylene, are fed into a packed bed reactor that is broken into five parts to allow for heat transfer for cooling. The product enters a separation train where the vapor products flue out of a flash tank. The liquid products enter two distillation columns in series to separate out acrylic acid first, and then acetic acid out the second. The remaining water after the second column is treated as waste water. The acrylic acid exits nearly 2,000 tonnes/year over production requirements at a purity of 99.9%. The acetic acid is purified to 95.3% and produces a little over 2,000 tonnes/year.

3 PROCESS FLOW DIAGRAM



4 PROCESS DESCRIPTION

The major goal of the process displayed in section 3 is to generate 50,000 tonnes of 99.9% pure Acrylic Acid per year. The secondary goal is to generate 95% pure Acetic Acid byproduct.

The reactor section begins with two input flows. One is propylene at 600 kPa, which is reduced to the reactor condition of 300 kPa (not modeled for brevity) and sent to a mixer to combine with the second feed. The second input is air, which is taken in from the atmosphere via compressor C-100 and pressurized to 300 kPa. The mixed stream then heated to reactor temperature and passes into a packed bed reactor operating at 250 °C. The reactor temperature was chosen for its high initial reaction rate and good selectivity of acrylic acid. The reactor geometry is five three-meter segments that are 1.4 meters in diameter, which allow for adequate cooling and allow the reactor to run isothermally. The high reactor pressure helps to drive the reaction to completion, resulting in a near 100% conversion of propylene to products. The products from the reactor are then flashed at 30 °C to give optimal separation of products from leftover reactants: oxygen, nitrogen, and propylene. These reactants are then sent to a flue to be burned as waste gas. The liquid products are reduced to 15 kPa in preparation for vacuum distillation. First the acrylic acid is separated from the acetic and water, which are sent to a second distillation column. This column separates the acetic acid from the water, which is then treated as wastewater. The two product streams were then pressurized and cooled to outlet conditions of 35°C and 1 atm.

The first unit modeled was C-100 which is an isentropic compressor that intakes air at atmospheric pressure and increases the pressure to 300 kPa. This compressed air is then mixed with propylene in M-100 to feed the reactor. The stream is also heated to 250 °C to match reactor conditions. This was not modeled in ASPEN for cleanliness of PFD; however, it was taken into account for heat integration which is explained later.

The Reactor (R-100) is a packed bed PFR which is loaded with 20,000 kg of catalyst and operates at 250 °C. The pressure was selected to drive the reaction to completion. 300 kPa was chosen as a pressure value where minimal reactant is left in the product stream as shown below:

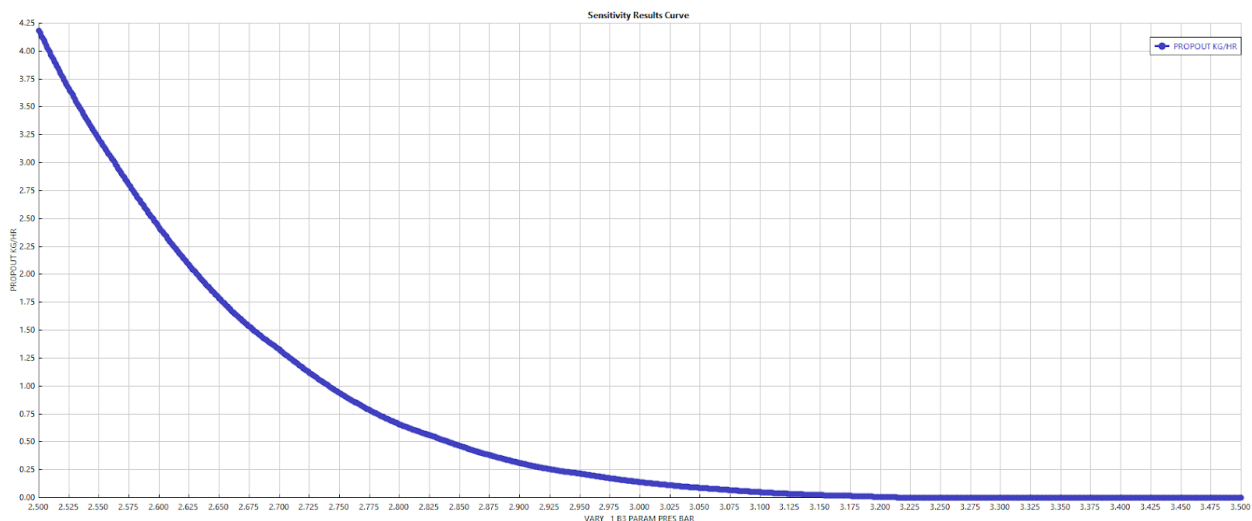
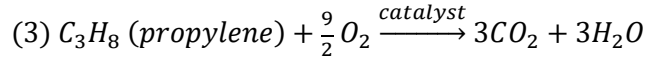
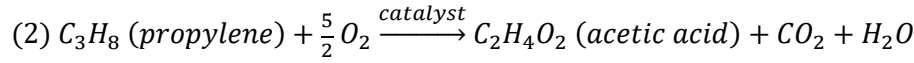
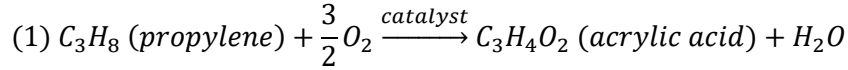


Figure 4.1: Sensitivity Analysis of Pressure vs Unreacted Propylene

Three reactions take place simultaneously in the reactor.



The reactions are first order in both propylene and oxygen, so the kinetics can be represented by the “powerlaw” reaction class and the general rate law:

$$r_i = k_i P_{C_3H_6} P_{O_2}$$

The selectivities from Table 1 in the problem statement were used to find the rate for each of the three reactions and subsequently the rate constant for each reaction. (Thio & Cuba-Torres, 2019) The Arrhenius equation was then used to estimate k and the activation energy for each reaction. These values were used in the reaction scheme in Aspen and are reproduced in the table below.

Reaction	k	E_a (kJ/mol)
1	3.3918	9.517
2	0.2445	9.259
3	603	59.08

Table 4.1: Reaction Kinetics

After R-100 the newly created products enter the separation train. First, they are condensed to 30 °C using a flash tank, V-100. The temperature was determined via sensitivity analysis.

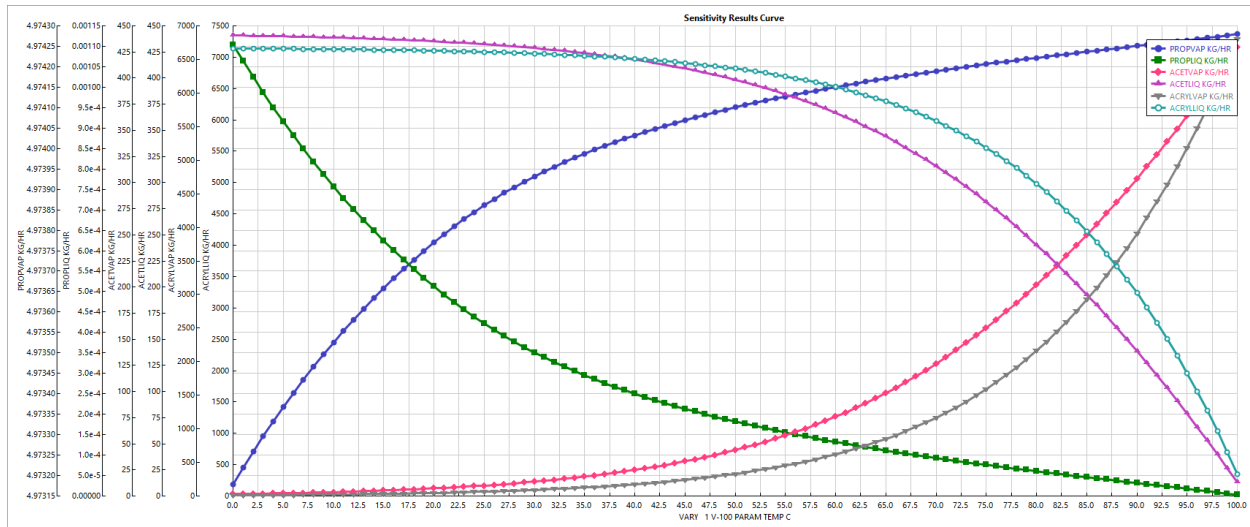


Figure 4.2: Sensitivity Analysis of V-100 Temperature vs Product quantities

Since the amount of propylene out of the reactor was so small, a recycle stream was determined to be unnecessary, and the effect of propylene on the sensitivity analysis was negligible. As a result, the decision of temperature was largely based on losing the least amount of salable product. 30 °C was a round number which was not too cold as to lead to unnecessary expense and fit well with the model.

After the flue gas was removed, the condensed product stream was depressurized to 15 kPa by the pump P-100 for vacuum distillation. The low-pressure product stream is then fed to tower T-100. This tower has 50 equilibrium stages, operates at a molar reflux ratio of 3.6, and feeds in on stage 8. The bottoms rate is set at 5,920 kg/hr. These values were determined by first modeling the tower as a DSTWU block, then optimizing values in Aspen until the desired separation was achieved. The bottoms stream from T-100 is product acrylic acid, which is then cooled and repressured to outlet conditions.

The distillate stream from T-100 is now composed of primarily water and acetic acid. That distillate is then fed to T-101 which has 33 equilibrium stages, operates at a molar reflux ratio of 2.9, and feeds in on stage 1. The bottoms rate is set at 240 kg/hr. These values were determined by first modeling the tower as a DSTWU block, then optimizing values in Aspen until the desired separation was achieved. The bottoms stream from T-101 is byproduct Acetic Acid and is cooled and repressured to outlet conditions. The distillate stream from T-101 is wastewater and is then processed as such.

To minimize the heat duties that were required, heat integration between the reactor and the reboilers of separation columns is conducted. Integration was calculated on paper, as it was determined to be easier than additional streams for the units modeled in Aspen. The outlet temperature of the reactor, run under adiabatic conditions, would have been 2,297 K. The C-value seen in the result stream tables below was calculated by multiplying the heat capacity of the mixture (C_p) and molar flow rate of that mixture to calculate the C in units (kJ/sec K). (see Appendix C for C of each units) Below is a temperature diagram representing the temperature intervals for the reactor, each reboiler of separation columns, and heat exchangers in question for heat integration. (see Appendix C for the heat duties of each intervals)

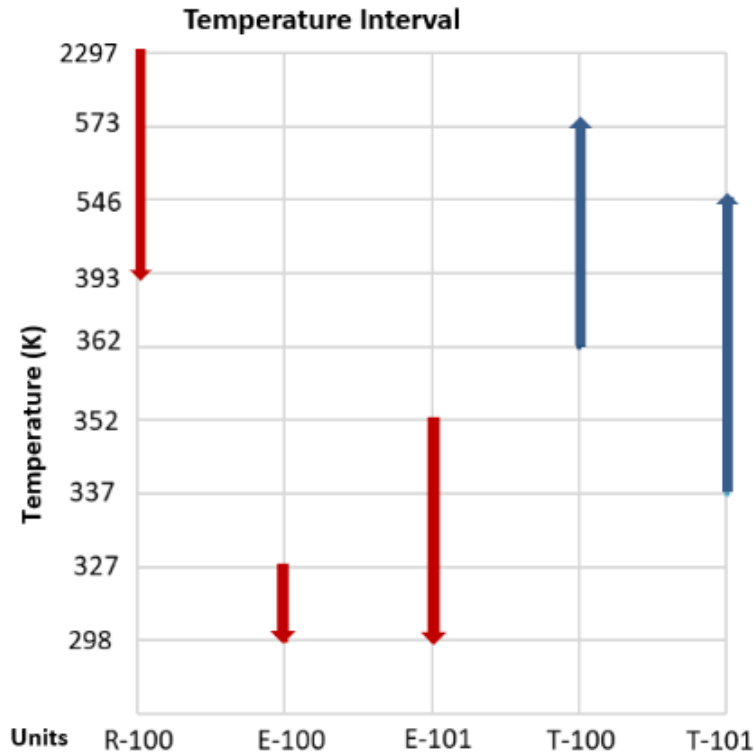


Figure 4.3: Temperature Intervals

The cold pinch temperature was found to be 337 K and a heat exchanger network was designed and drawn below. Heat coming from the exothermic reaction in the reactor can be integrated to both the reboilers of the separation columns and it satisfies the condition above the pinch temperature $C_C > C_H$, as well as the required heat duties. An additional heat duty of 15,726 kW is to be removed after the heat integration. Both heat exchangers still require their cooling duties for their condensers.

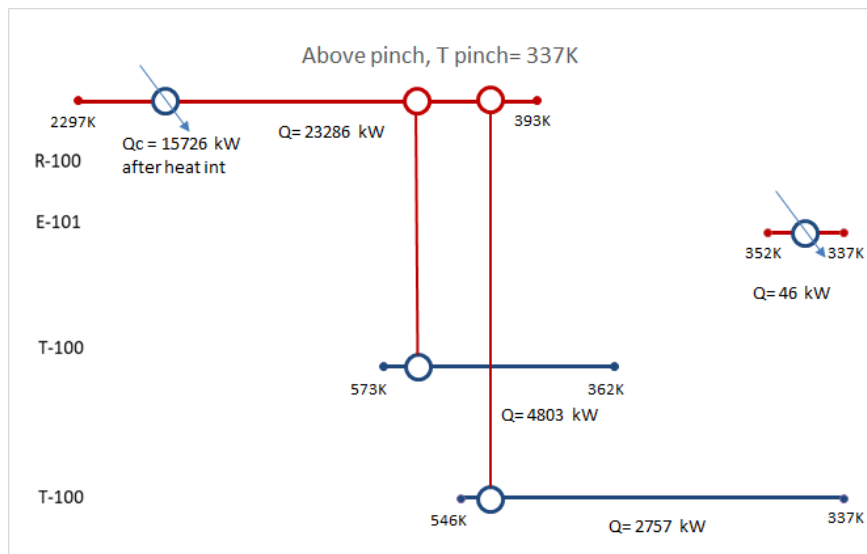


Figure 4.4: Integration Diagram above Pinch Point

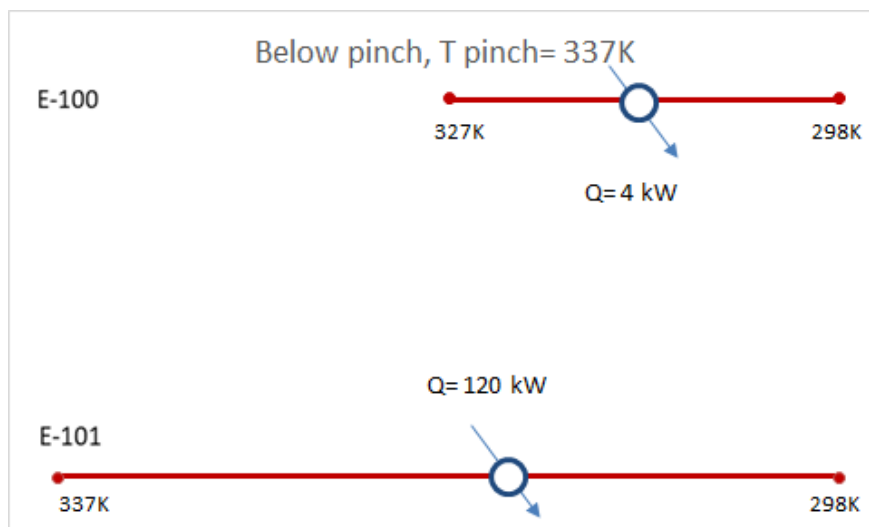


Figure 4.5: Integration Diagram below Pinch Point.

These heat exchangers were not modeled in Aspen for clarity and ease of calculation; however, they were considered for all economic calculations.

5 ENERGY BALANCE AND COSTS

Cooling

Unit Operation	Requirement	Magnitude (kJ/hr)	Magnitude After Heat Integration (kJ/hr)	Flow (kg/hr)	Temperature Change	Annual Utility Cost (\$/year)
E-100	Cooling	-1.41E+04	-1.41E+04	240	64°C --> 35°C	\$ 5.88
E-101	Cooling	-5.57E+05	-5.57E+05	5,921	88°C --> 35°C	\$ 425.00

Phase Change

Unit Operation	Requirement	Magnitude (kJ/hr)	Magnitude After Heat Integration (kJ/hr)	Flow (kg/hr)	Phase Change	Annual Utility Cost (\$/year)
T-100	Condenser	-1.29E+07	-1.29E+07	1,811	V --> L	\$ 39,100.00
T-100	Reboiler	1.73E+07	-	5,921	L --> V	\$ -
T-101	Condenser	-2.02E+07	-2.02E+07	1,571	V --> L	\$ 60,800.00
T-101	Reboiler	9.93E+06	-	240	L --> V	\$ -

Pressure Change

Unit Operation	Requirement	Magnitude (kJ/hr)	Magnitude After Heat Integration (kJ/hr)	Flow (kg/hr)	Pressure Change	Annual Utility Cost (\$/year)
C-100	Compressor	5.39E+06	5.39E+06	32,785	101kPa --> 300 kPa	\$ 838,000.00
P-100	Pump	1.63E+03	1.63E+03	7,732	300kPa --> 15kPa	\$ 254.00
P-101	Pump	1.53E+03	1.53E+03	5,921	15kPa --> 101kPa	\$ 238.00
P-102	Pump	6.90E+01	6.90E+01	240	15kPa --> 101kPa	\$ 11.00

Reactors

Unit Operation	Requirement	Magnitude (kJ/hr)	Magnitude After Heat Integration (kJ/hr)	Flow (kg/hr)	Temperature Change	Annual Utility Cost (\$/year)
R-100	Cooling	-5.78E+07	-3.06E+07	36,573	250°C --> 250°C	\$ 559,000.00

6 ECONOMIC ANALYSIS

UO	UO Type	Dimensions	Vol. Flowrate (m ³ /hr)	Transfer Area (m ²)	Power/ Duty (kW)	Item Cost (C _p)	Bare Module Cost (C _{bm})
C-100	Compressor	-	29,133.38	-	1,496.46	\$ 1,043,300.00	\$ 1,359,200.00
M-100	Mixer	-	-	-	-	\$ -	\$ -
R-100	Reactor	d=1.4m, L=15m	-	-	-	\$ 82,200.00	\$ 245,600.00
V-100	Flash Tank	-	-	-	-	\$ 24,300.00	\$ 147,200.00
P-100	Pump	-	8.30	-	-0.45	\$ 5,600.00	\$ 36,500.00
T-100	Separation Col.	-	-	-	-	\$ 1,527,800.00	\$ 2,586,100.00
	Bottoms split	-	-	-	-	\$ -	\$ -
	Condenser	-	-	195.63	3,578.00	\$ 41,700.00	\$ 137,900.00
	Cond acc	-	-	-	-	\$ 11,700.00	\$ 81,100.00
	Overhead split	-	-	-	-	\$ -	\$ -
	Reboiler	-	-	104.46	4,809.87	\$ 38,000.00	\$ 142,500.00
	Reflux Pump	-	7.92	-	-	\$ 5,600.00	\$ 36,500.00
	Tower	-	-	-	-	\$ 1,430,800.00	\$ 2,188,100.00
P-101	Pump	-	6.69	-	0.42	\$ 4,900.00	\$ 35,800.00
E-104	Heater	-	-	15.20	154.00	\$ 11,500.00	\$ 81,600.00
T-101	Separation Col.	-	-	-	-	\$ 748,600.00	\$ 1,573,100.00
	Bottoms split	-	-	-	-	\$ -	\$ -
	Condenser	-	-	155.16	2,793.00	\$ 36,100.00	\$ 131,800.00
	Cond acc	-	-	-	-	\$ 16,500.00	\$ 106,300.00
	Overhead split	-	-	-	-	\$ -	\$ -
	Reboiler	-	-	35.99	2,759.39	\$ 21,800.00	\$ 110,500.00
	Reflux Pump	-	5.42	-	-	\$ 5,500.00	\$ 35,000.00
	Tower	-	-	-	-	\$ 668,700.00	\$ 1,189,500.00
P-102	Pump	-	-	-	0.02	\$ 4,300.00	\$ 28,900.00
E-105	Heater	-	-	0.45	3.90	\$ 8,400.00	\$ 54,200.00
P-103	Pump	-	92.36	-	0.62	\$ 7,800.00	\$ 51,500.00
Total Costs						\$ 5,745,100.00	\$ 10,358,900.00

Table 6.1: Purchase and Bare-Module Costs for Equipment

All bare module costs were determined by utilizing the ASPEN economics analysis tool. All relevant dimensions and specifications listed in the table above were also determined utilizing ASPEN mapping and sizing tools. For heat exchangers, the transfer area (m^2) and the heat duty (kW), are reported, as seen above. All compressors and pumps list the volumetric flow rate (m^3/hr) and power required (kW) in the table above. The dimension of the reactor was a big optimization challenge in this phase of the project, because the surface area had to be increased to keep the reactor isothermal. To overcome this challenge, it was decided to split the reactor into 5 three-meter segments with a diameter of 1.4 meters. All the bare module costs listed in Table 6.1 were summed and included in the total capital investment cost sheet, seen below.

Capital Investment Calculations		
C_{FE}	\$ 8,775,500.00	Fabricated equipment
C_{PM}	\$ 1,531,900.00	Process machinery
C_{spare}	\$ 11,200.00	2 spares for Pumps
$C_{storage}$	\$ 201,980.00	48 hr storage
C_{comp}	\$ -	
$C_{catalyst}$	\$ 200,000.00	20,000 kg catalyst/yr
C_{TBM}	\$ 10,720,580.00	
C_{site}	\$ 536,029.00	5% C_{TBM}
C_{serv}	\$ 268,014.50	5% C_{site}
C_{alloc}	\$ -	No Allocated costs
C_{DPI}	\$ 11,524,623.50	
C_{cont}	\$ 1,152,462.35	10% C_{DPI}
C_{TDC}	\$ 12,677,085.85	
C_{land}	\$ -	
C_{royal}	\$ -	
$C_{startup}$	\$ 1,267,708.59	10% C_{TDC}
C_{TPI}	\$ 13,944,794.44	
C_{WC}	\$ 27,200,946.42	
C_{TCI}	\$ 41,145,740.85	

Table 6.2: Calculations of Capital Cost

When calculating the cost of the total capital investment (C_{TCI}), several assumptions were made based on the heuristics of the textbook⁶. For the cost of spares (C_{spare}), liquid pumps are mainly considered since spares for compressors are too expensive to have on hand without immediate usage. In this plant there are three liquid pumps of three different sizes, therefore the cost of spares was calculated based on the bare module cost of the most expensive pump. Based on the ASPEN economics tool the cost for the most expensive pump was of \$5,600, multiplied by two for a total of \$11,200.

For the cost of storage ($C_{storage}$), all calculations for the bare module cost of each tank are shown in Appendix A. The size of the tanks was based on 48 hours of liquid output. A cone-roof tank was chosen based on the output volume and pressure of product acetic and acrylic acid streams. An open tank would be a cheaper option, but not ideal due to it being exposed to rain, which could affect the purity of our products, negatively impacting sales. After determining the type and size of the tanks, the bare module factor (Table 16.11), was used to consider the installation costs and obtain the final bare module costs.⁶ The

FBM utilized was that of a crystallizer, with a value of 2.06. Given the functionality of a crystallizer is relatively similar to that of a storage tank, it was deemed the most accurate option for costing the storage tanks. Finally, the bare module costs of both tanks were added resulting in the final storage cost of \$201,980.

For the catalyst cost was found to be \$200,000 per year, based on the requirement that all 20,000kg of catalyst be replaced on a yearly basis. The costs for the fabricated equipment and process machinery (C_{FE} , C_{PM}), were simply the sum of the bare module costs shown in Table 6.1. No accurate heuristic was found for calculating the cost of computers and software so it was left blank on the table above. Based on other plants the cost of computers and software is low compared to the other costs, meaning it could likely be neglected without hindering the final economic analysis.

Finally, all these costs were summed resulting in a total bare-module cost (C_{TBM}) of \$10,720,580. This value was then used to calculate the total capital investment (C_{TCI}) by following the heuristics of the cost sheet. The value for the cost of working capital (C_{WC}) is equivalent to half of the total production cost, excluding depreciation. The calculations done in every step of the process from the total bare module cost all the way to the total capital invested can be seen in the comments section of Table 6.2. The total capital investment needed for the first year to build the entire plant was of \$41,145,740.

All the calculations for the total production cost, seen in Table 6.3, were based on Table 17.1 of the textbook.⁶ Most of the calculations for each step can be seen in the comments section of the table above. DWS&B was calculated based on Table 17.3 of the textbook⁶, and shows a continuous operation fluids process requires one operator per process section. The plant was subdivided into three process sections, one for the reactor system and two different separation sections, one for each distillation column. The final value of DWS&B was calculated assuming 5 shifts/week and 8000 hours of production per year. It was also assumed the new plant needed one technical assistance and one control lab workers. This was multiplied by 5 shifts, and then multiplied by the price given in Table 17.1, resulting in \$300,000 and \$325,000 for technical assistance and control laboratory, respectively. All calculations for the feedstock costs are shown in detail in the Appendix A. The final production cost was of \$54,401,893.

Section	Costs	Comments
Feedstock		
Propylene	\$ 34,539,720.00	Price: \$1,140/ metric ton
Utilities (electricity)	\$ 4,494,541.27	
Cooling Water	\$ 17,340.48	
Wastewater Treatment	\$ 389,520.00	
Operations (Labor Related)		
DW&B	\$ 1,248,000.00	\$40/operator-hr
DS&B	\$ 187,200.00	15% of DW&B
Op Supplies/Services	\$ 74,880.00	6% of DW&B
Tech assist (1)	\$ 300,000.00	\$60,000/(operator/shift)-yr
Control Lab (1)	\$ 325,000.00	\$65,000/(operator/shift)-yr
Maintenance		
MW&B (fluids processing)	\$ 443,698.00	3.5% of CTDC
S&B	\$ 110,924.50	25% of MW&B
Materials and Services	\$ 443,698.00	100% of MW&B
Maintenance Overhead	\$ 22,184.90	5% of MW&B
Operation Overhead		
Gen Plant Overhead	\$ 141,277.40	7.1% of M&O-SW&B
Mechanical Dept. Services	\$ 47,755.74	2.4% of M&O-SW&B
Employee Relations Dept.	\$ 117,399.53	5.9% of M&O-SW&B
Business Services	\$ 147,246.87	7.4% of M&O-SW&B
Property Taxes and Insurance	\$ 253,541.72	2% of CTDC
COM	\$ 43,303,928.41	Sum of Above
General Expenses (GE)		
Selling Expense	\$ 2,882,588.16	3% of sales
Direct Research	\$ 4,612,141.06	4.8% of sales
Allocated Research	\$ 480,431.36	0.5% of sales
Adm Expenses	\$ 1,921,725.44	2.0% of sales
Management Incentive	\$ 1,201,078.40	1.25% of sales
GE	\$ 11,097,964.42	Sum of above
Total Production Cost	\$ 54,401,892.83	GE + COM

Table 6.3: Calculations for Total Production Costs

Tax Rate		26%						
Inflation		2%						
Interest Rate		15%						
Year	TCI	Sales	Depreciation	Cost (minus D)	Cost	Salvage	CF	Discounted CF
2020 - 0	\$ 41,145,741	\$ -	\$ -	\$ -	\$ -	\$ -	\$(41,145,741)	\$ (41,145,741)
2021 - 1	\$ -	\$ 96,086,272	\$ 4,114,574	\$ 50,287,319	\$ 54,401,893	\$ -	\$ 38,005,799	\$ 33,637,934
2022 - 2	\$ -	\$ 96,086,272	\$ 7,406,233	\$ 46,995,659	\$ 54,401,893	\$ -	\$ 43,733,287	\$ 34,178,374
2023 - 3	\$ -	\$ 96,086,272	\$ 5,924,987	\$ 48,476,906	\$ 54,401,893	\$ -	\$ 41,155,917	\$ 28,478,562
2024 - 4	\$ -	\$ 96,086,272	\$ 4,739,989	\$ 49,661,903	\$ 54,401,893	\$ -	\$ 39,094,022	\$ 23,971,269
2025 - 5	\$ -	\$ 96,086,272	\$ 3,793,637	\$ 50,608,256	\$ 54,401,893	\$ -	\$ 37,447,370	\$ 20,359,426
2026 - 6	\$ -	\$ 96,086,272	\$ 3,032,441	\$ 51,369,452	\$ 54,401,893	\$ -	\$ 36,122,888	\$ 17,421,790
2027 - 7	\$ -	\$ 96,086,272	\$ 2,695,046	\$ 51,706,847	\$ 54,401,893	\$ -	\$ 35,535,821	\$ 15,194,914
2028 - 8	\$ -	\$ 96,086,272	\$ 2,695,046	\$ 51,706,847	\$ 54,401,893	\$ -	\$ 35,535,821	\$ 13,459,608
2029 - 9	\$ -	\$ 96,086,272	\$ 2,699,161	\$ 51,702,732	\$ 54,401,893	\$ -	\$ 35,542,980	\$ 11,924,969
2030 - 10	\$ -	\$ 96,086,272	\$ 2,695,046	\$ 51,706,847	\$ 54,401,893	\$ 633,854	\$ 36,169,675	\$ 10,752,641
							NPV	\$ 168,233,745.02

Table 6.4: Cash Flow Spreadsheet with NPV at 15% Interest Rate

The NPV for the process was calculated by using the MACRS model of depreciation for a period of 10 years of operation. The advantage of the MACRS model is that it combines characteristics from the straight-line and declining-balance models, giving a wholesome estimation of the future value of the investment. A Tax rate of 26%, inflation rate of 2%, and interest rate of 15% were utilized to calculate the cash flow for the plant. All formulas utilized in the excel code to calculate the NPV are shown in Appendix A. The final NPV value was of \$168,233,745, suggesting the plant is a good investment based on this modeling.

Tax Rate		26%						
Inflation		2%						
Interest Rate		99.76%						
Year	TCI	Sales	Depreciation	Cost (minus D)	Cost	Salvage	CF	Discounted CF
2020 - 0	\$ 41,145,741	\$ -	\$ -	\$ -	\$ -	\$ -	\$(41,145,741)	\$ (41,145,741)
2021 - 1	\$ -	\$ 96,086,272	\$ 4,051,189	\$ 50,350,704	\$ 54,401,893	\$ -	\$ 37,895,509	\$ 19,309,369
2022 - 2	\$ -	\$ 96,086,272	\$ 7,292,140	\$ 47,109,753	\$ 54,401,893	\$ -	\$ 43,534,763	\$ 11,276,789
2023 - 3	\$ -	\$ 96,086,272	\$ 5,833,712	\$ 48,568,181	\$ 54,401,893	\$ -	\$ 40,997,099	\$ 5,413,136
2024 - 4	\$ -	\$ 96,086,272	\$ 4,666,969	\$ 49,734,924	\$ 54,401,893	\$ -	\$ 38,966,967	\$ 2,624,725
2025 - 5	\$ -	\$ 96,086,272	\$ 3,735,196	\$ 50,666,697	\$ 54,401,893	\$ -	\$ 37,345,682	\$ 1,284,057
2026 - 6	\$ -	\$ 96,086,272	\$ 2,985,726	\$ 51,416,167	\$ 54,401,893	\$ -	\$ 36,041,604	\$ 632,856
2027 - 7	\$ -	\$ 96,086,272	\$ 2,653,529	\$ 51,748,364	\$ 54,401,893	\$ -	\$ 35,463,580	\$ 317,832
2028 - 8	\$ -	\$ 96,086,272	\$ 2,653,529	\$ 51,748,364	\$ 54,401,893	\$ -	\$ 35,463,580	\$ 162,080
2029 - 9	\$ -	\$ 96,086,272	\$ 2,657,580	\$ 51,744,313	\$ 54,401,893	\$ -	\$ 35,470,629	\$ 82,670
2030 - 10	\$ -	\$ 96,086,272	\$ 2,653,529	\$ 51,748,364	\$ 54,401,893	\$ 633,854	\$ 36,097,435	\$ 42,916
							NPV	\$ -

Table 6.5: Cashflow Spreadsheet with IRR Calculation

The IRR was of 99.76%, and it was determined by utilizing the previous cash flow spreadsheet in combination with Excel SOLVER. The NPV value was set to a goal of zero, while changing the IRR cell. This enabled us to determine what would be the IRR where the NPV value would be zero. An investor's rate of return (IRR) of 99.76% is very high, which makes sense based on the high NPV value. The higher the IRR the better the return on the investment, reinforcing that this process stands to be extremely profitable over a 10-year lifetime.

Tax Rate	26%							
Inflation	2%							
Interest Rate	15%							
Year	TCI	Sales	Depreciation	Cost (minus D)	Cost	Salvage	CF	Discounted CF
2020 - 0	\$ 40,895,741	\$ -	\$ -	\$ -	\$ -	\$ -	\$(40,895,741)	\$ (40,895,741)
2021 - 1	\$ -	\$ 96,086,272	\$ 4,026,189	\$ 92,027,872	\$ 96,054,060	\$ -	\$ 7,029,405	\$ 6,164,756
2022 - 2	\$ -	\$ 96,086,272	\$ 7,247,140	\$ 88,806,921	\$ 96,054,060	\$ -	\$ 12,633,859	\$ 9,717,567
2023 - 3	\$ -	\$ 96,086,272	\$ 5,797,712	\$ 90,256,349	\$ 96,054,060	\$ -	\$ 10,111,855	\$ 6,822,333
2024 - 4	\$ -	\$ 96,086,272	\$ 4,638,169	\$ 91,415,891	\$ 96,054,060	\$ -	\$ 8,094,251	\$ 4,790,803
2025 - 5	\$ -	\$ 96,086,272	\$ 3,712,146	\$ 92,341,914	\$ 96,054,060	\$ -	\$ 6,482,971	\$ 3,366,563
2026 - 6	\$ -	\$ 96,086,272	\$ 2,967,301	\$ 93,086,759	\$ 96,054,060	\$ -	\$ 5,186,940	\$ 2,363,524
2027 - 7	\$ -	\$ 96,086,272	\$ 2,637,154	\$ 93,416,907	\$ 96,054,060	\$ -	\$ 4,612,484	\$ 1,844,417
2028 - 8	\$ -	\$ 96,086,272	\$ 2,637,154	\$ 93,416,907	\$ 96,054,060	\$ -	\$ 4,612,484	\$ 1,618,676
2029 - 9	\$ -	\$ 96,086,272	\$ 2,641,180	\$ 93,412,881	\$ 96,054,060	\$ -	\$ 4,619,489	\$ 1,422,859
2030 - 10	\$ -	\$ 96,086,272	\$ 2,637,154	\$ 93,416,907	\$ 96,054,060	\$ 633,854	\$ 5,246,338	\$ 1,438,055
NPV								\$ -
New Propylene Price (per Metric Ton)								\$ 2,504.00

Table 6.6: Calculation of New Propylene Price with IRR of 15%

For this final economic analysis calculation, a hypothetical propylene price was determined for an IRR of 15%. For this calculation a similar cash flow spreadsheet was utilized as seen in Table 6. Excel solver was utilized, by setting the goal of the IRR cell to 15% and NPV to zero, while changing the original price of propylene given of \$1,140/metric ton. After running the SOLVER, the new price of propylene is of \$2,504 per metric ton. The price is roughly double of the original, which makes sense based off the high values for original IRR and NPV and suggests that the plant is a sturdy investment.

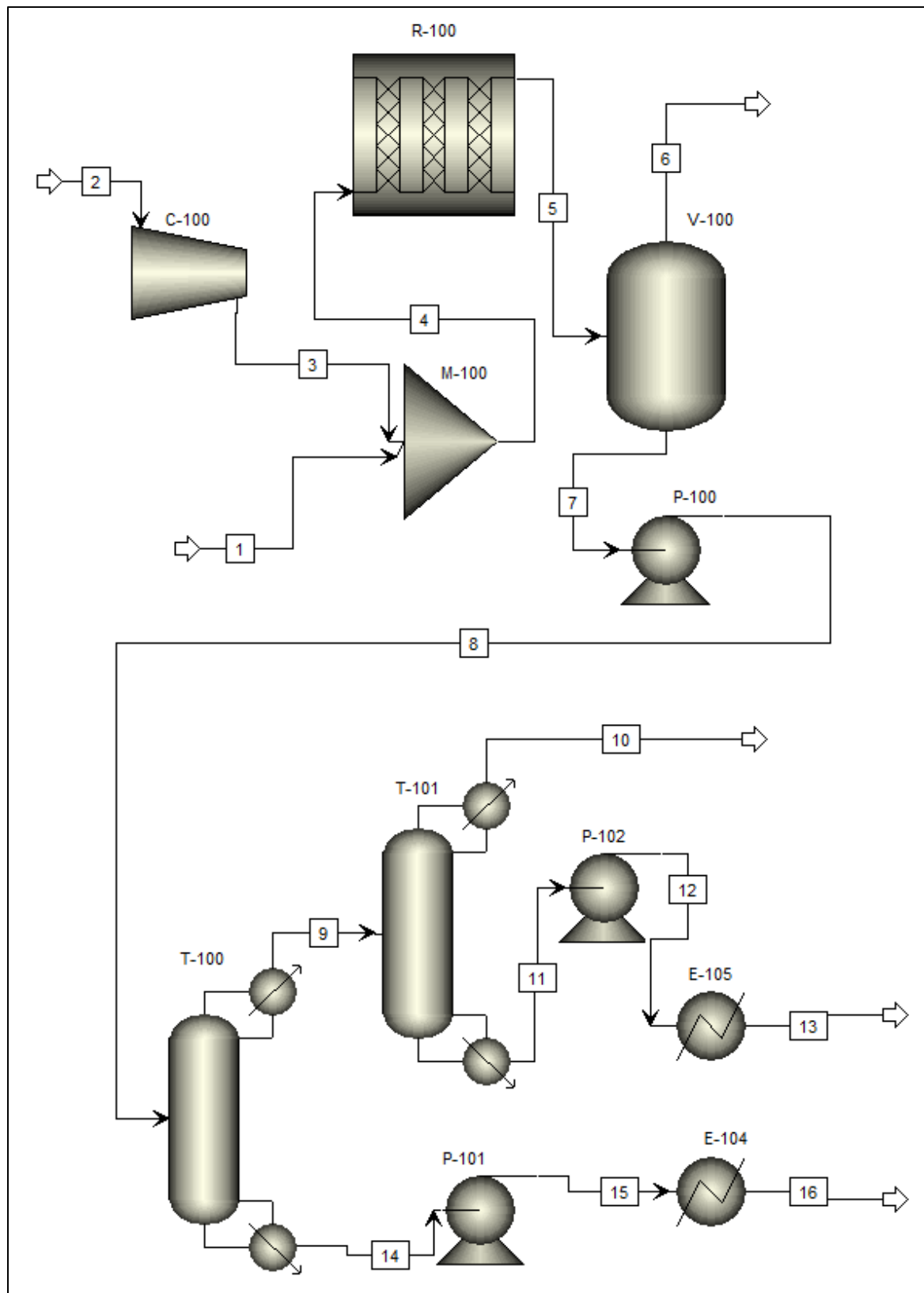
7 CONCLUSIONS AND RECOMMENDATIONS

The choice to produce acrylic acid via oxidation of propylene was made based on a promising profit upper bound of \$410-1,220 per tonne and the simplicity of reaction and separation process that route offered. Though the process has a few drawbacks, primarily safety related, most could be solved by proper industrial hygiene and plant safety. The process modeling showed that, in order to produce 51,900 tonne/year of acrylic acid at 99.9% purity, 33,199 tonne/year of propylene and 287,400 tonne/year of air are required to be reacted in five 3-meter reactor segments in series operating at 250 °C, with a total of 20,000 kg of catalyst and residence time of 81.6 seconds. This product is fed into a separation train of one flash drum and two distillation columns. The entire process produces a net 3,230 kJ/h before heat integration. A side product of 95.3% pure acetic acid is produced and collected at a rate of 2,056 tonne/year.

The major source of energy consumption of the process were the two separation columns and the compressor at the start of the process. While the compressor is necessary to force air into the mixer, the process may have been more efficient if a valve was used to depressurize the propylene to a lower level so that the compressor would not require so much energy to pump the air to as high a pressure. Oxygen should be considered to replace air, as it would make the compressor volumetric flow about a fifth of what is currently is, while not wasting reactor space on nitrogen. The separation energy costs were offset by heat integrating the reaction heat to the reboilers, saving 7.5 MW that was previously required, and saving over \$4 million per year. Another aspect that could be optimized is the amount of catalyst used, which in the simulation was 20,000kg. This number was used because increasing the weight did not significantly improve the reaction conversion, while decreasing it saw noticeable changes in product production. The final value used for weight was rounded up to ensure enough catalyst for reaction.

When the reactor was designed, a recycle was considered, but was deemed unnecessary due to the amount of propylene out of the reactor being only 0.3 tonnes/year. It was more efficient to flue the leftover reactant than to try to separate it, which was deemed too expensive for such a small amount, less than a thousandth of a percent of the original input. With this being said, the reactor required is fairly large, requiring 23 m³ volume and 20,000kg of catalyst. The group recommends that an alternative reactor be explored that considers a smaller reactor that does not react all the propylene but has a recycle to compensate. The smaller reactor design could be paired with using oxygen instead of air. As mentioned before, this would reduce the volumetric need for the reactor, as currently, nearly 70% of the mass moving through the reactor is nitrogen. Removing it should help propylene and oxygen to better mix and react, though no analysis nor research have been done to support this and proper examination of this process is required before moving forward. This alternative would require a smaller reactor (and therefore less space), less catalyst, and will require significantly less water for cooling. While less water would cost less in utilities and require a less expensive pump to operate the cooling flow, it would leave less energy for heat integration to the reboilers. Further analysis should be done to find the minimum water flow that would satisfy the reboiler energy needs.

8 MATERIAL BALANCES



Stream	1	2	3	4
Phase	Vapor	Vapor	Vapor	Vapor
Temperature (°C)	30.0	30.0	147.3	121.2
Pressure (kPa)	600.0	101.3	300.0	300.0
Enthalpy Flow (kJ/hr)	1.794E+06	-4.931E+05	3.278E+06	5.072E+06
Volume Flow (L/sec)	96.63	7,356.92	3,450.79	3,563.94
Mole Flows (kmol/hr)	90.00	1,136.40	1,136.40	1,226.40
Propylene	90.00	-	-	90.00
Acrylic Acid	-	-	-	-
Acetic Acid	-	-	-	-
Carbon Dioxide	-	-	-	-
Water	-	-	-	-
Oxygen	-	238.64	238.64	238.64
Nitrogen	-	897.76	897.76	897.76
Mole Fractions				
Propylene	1.00	-	-	0.07
Acrylic Acid	-	-	-	-
Acetic Acid	-	-	-	-
Carbon Dioxide	-	-	-	-
Water	-	-	-	-
Oxygen	-	0.21	0.21	0.19
Nitrogen	-	0.79	0.79	0.73
Mass Flows (kg/hr)	3,787.26	32,785.71	32,785.71	36,572.96
Propylene	3,787.26	-	-	3,787.26
Acrylic Acid	-	-	-	-
Acetic Acid	-	-	-	-
Carbon Dioxide	-	-	-	-
Water	-	-	-	-
Oxygen	-	7,636.35	7,636.35	7,636.35
Nitrogen	-	25,149.36	25,149.36	25,149.36
Mass Fractions				
Propylene	1.00	-	-	0.10
Acrylic Acid	-	-	-	-
Acetic Acid	-	-	-	-
Carbon Dioxide	-	-	-	-
Water	-	-	-	-
Oxygen	-	0.23	0.23	0.21
Nitrogen	-	0.77	0.77	0.69

(continued...)

Stream	5	6	7	8
Phase	Vapor	Vapor	Liquid	Liquid
Temperature (°C)	250.0	30.0	30.0	30.0
Pressure (kPa)	300.0	300.0	300.0	15.0
Enthalpy Flow (kJ/hr)	-4.654E+07	-6.076E+06	-5.831E+07	-5.831E+07
Volume Flow (L/sec)	4,678.59	2,110.37	2.11	2.11
Mole Flows (kmol/hr)	1,181.57	1,011.22	170.35	170.35
Propylene	-	-	-	-
Acrylic Acid	83.41	1.18	82.23	82.23
Acetic Acid	6.42	0.21	6.21	6.21
Carbon Dioxide	6.92	6.92	-	-
Water	90.34	8.44	81.89	81.89
Oxygen	96.72	96.72	-	-
Nitrogen	897.76	897.75	0.01	0.01
Mole Fractions				
Propylene	-	-	-	-
Acrylic Acid	0.07	-	0.48	0.48
Acetic Acid	0.01	-	0.04	0.04
Carbon Dioxide	0.01	0.01	-	-
Water	0.08	0.01	0.48	0.48
Oxygen	0.08	0.10	-	-
Nitrogen	0.76	0.89	-	-
Mass Flows (kg/hr)	36,572.99	28,798.49	7,774.50	7,774.50
Propylene	-	-	-	-
Acrylic Acid	6,011.01	85.29	5,925.72	5,925.72
Acetic Acid	385.54	12.62	372.92	372.92
Carbon Dioxide	304.72	304.51	0.20	0.20
Water	1,627.44	152.13	1,475.30	1,475.30
Oxygen	3,094.93	3,094.84	0.08	0.08
Nitrogen	25,149.36	25,149.08	0.27	0.27
Mass Fractions				
Propylene	-	-	-	-
Acrylic Acid	0.16	-	0.76	0.76
Acetic Acid	0.01	-	0.05	0.05
Carbon Dioxide	0.01	0.01	-	-
Water	0.04	0.01	0.19	0.19
Oxygen	0.08	0.11	-	-
Nitrogen	0.69	0.87	-	-

(continued...)

Stream	9	10	11	12
Phase	Vapor	Vapor	Liquid	Liquid
Temperature (°C)	54.7	54.4	65.7	65.8
Pressure (kPa)	15.0	15.0	15.0	101.3
Enthalpy Flow (kJ/hr)	-2.252E+07	-2.074E+07	-1.896E+06	-1.896E+06
Volume Flow (L/sec)	4,342.19	4,198.25	0.07	0.07
Mole Flows (kmol/hr)	88.18	84.19	4.00	4.00
Propylene	-	-	-	-
Acrylic Acid	0.12	0.02	0.10	0.10
Acetic Acid	6.15	2.28	3.87	3.87
Carbon Dioxide	-	-	-	-
Water	81.89	81.87	0.03	0.03
Oxygen	-	-	-	-
Nitrogen	0.01	0.01	-	-
Mole Fractions				
Propylene	-	-	-	-
Acrylic Acid	-	-	0.02	0.02
Acetic Acid	0.07	0.03	0.97	0.97
Carbon Dioxide	-	-	-	-
Water	0.93	0.97	0.01	0.01
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Mass Flows (kg/hr)	1,853.90	1,613.90	240.00	240.00
Propylene	-	-	-	-
Acrylic Acid	8.55	1.44	7.11	7.11
Acetic Acid	369.49	137.07	232.42	232.42
Carbon Dioxide	0.20	0.20	-	-
Water	1,475.30	1,474.83	0.47	0.47
Oxygen	0.08	0.08	-	-
Nitrogen	0.27	0.27	-	-
Mass Fractions				
Propylene	-	-	-	-
Acrylic Acid	-	-	0.03	0.03
Acetic Acid	0.20	0.08	0.97	0.97
Carbon Dioxide	-	-	-	-
Water	0.80	0.91	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-

(continued...)

Stream	13	14	15	16
Phase	Liquid	Liquid	Liquid	Liquid
Temperature (°C)	35.0	88.2	88.3	35.0
Pressure (kPa)	101.3	15.0	101.3	101.3
Enthalpy Flow (kJ/hr)	-1.911E+06	-3.125E+07	-3.125E+07	-3.181E+07
Volume Flow (L/sec)	0.06	1.69	1.69	1.59
Mole Flows (kmol/hr)	4.00	82.17	82.17	82.17
Propylene	-	-	-	-
Acrylic Acid	0.10	82.11	82.11	82.11
Acetic Acid	3.87	0.06	0.06	0.06
Carbon Dioxide	-	-	-	-
Water	0.03	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Mole Fractions				
Propylene	-	-	-	-
Acrylic Acid	0.02	1.00	1.00	1.00
Acetic Acid	0.97	-	-	-
Carbon Dioxide	-	-	-	-
Water	0.01	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Mass Flows (kg/hr)	240.00	5,920.60	5,920.60	5,920.60
Propylene	-	-	-	-
Acrylic Acid	7.11	5,917.17	5,917.17	5,917.17
Acetic Acid	232.42	3.43	3.43	3.43
Carbon Dioxide	-	-	-	-
Water	0.47	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-
Mass Fractions				
Propylene	-	-	-	-
Acrylic Acid	0.03	1.00	1.00	1.00
Acetic Acid	0.97	-	-	-
Carbon Dioxide	-	-	-	-
Water	-	-	-	-
Oxygen	-	-	-	-
Nitrogen	-	-	-	-

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10 APPENDIX A – ECONOMIC ANALYSIS CALCULATIONS

10.1 BARE MODULE COST

Storage tanks require 48hr of storage for Acrylic Acid and Acetic Acid.

Acrylic Acid:

$$5920 \frac{kg}{hr} \cdot 48hr = 284,160kg$$

$$284,160kg \cdot \left(\frac{1m^3}{1050kg} \right) \cdot \left(\frac{264.17gal}{1m^3} \right) = 71,492gal$$

From Table 16.32 - Cone Roof Storage Tank

$$C_p = 265 \cdot (71,492)^{0.513} = \$81,936$$

From Table 16.11 – Crystallizer $F_{BM} = 2.06$

$$C_{BM} = \$81,936 \cdot 2.06 \approx \boxed{\$168,800}$$

Acetic Acid:

$$240 \frac{kg}{hr} \cdot 48hr = 11,520kg$$

$$11,520kg \cdot \left(\frac{1m^3}{1050kg} \right) \cdot \left(\frac{246.17gal}{1m^3} \right) = 2,898gal$$

From Table 16.32 – Cone Roof Storage Tank

$$C_p = 265 \cdot (2,898)^{0.513} = \$16,107$$

From Table 16.11 – Crystallizer $F_{BM} = 2.06$

$$C_{BM} = \$16,107 \cdot 2.06 \approx \boxed{\$33,180}$$

Total Storage

$$C_{storage} = \$168,800 + \$33,180 = \boxed{\$201,980}$$

10.2 FEED STOCK CALCULATIONS FOR TOTAL PRODUCTION COST

Propylene Feed Cost:

$$3,787 \frac{kg}{hr} \cdot 8,000 \frac{hrs}{yr} \cdot 0.001 \frac{tonne}{kg} \cdot \frac{\$1,140}{tonne} = \boxed{\$34,539,000/year}$$

Waste Water Treatment:

$$147.535 \frac{kg}{hr} \cdot \frac{\$0.33}{kg \text{ organic removed}} \cdot 8000 \frac{hr}{yr} = \boxed{\$389,520/year}$$

Cooling Water for Reactor:

$$\text{Cooling water flow} = 80.28 \text{ m}^3/\text{hr} \cdot 8000 \text{ hrs/yr} \cdot \$0.027/\text{m}^3 = \$17,340$$

10.3 CASH FLOW SPREADSHEET FORMULAE

Cash Flow (CF):

$$CF = (1 - t) \cdot (s - c) + D - f \cdot C_{TDI} + S_v$$

Discounted Cash Flow (DCF):

$$DCF = (CF - D) \cdot \frac{(1 + f)^k}{(1 + i)^k} + \frac{D}{(1 + i)^k}$$

Net Present Value (NPV):

$$NPV = \sum DCF$$

11 APPENDIX B – REACTOR KINETICS

Based on the information given in Table 1 of the problem statement, the general rate law for all three of the reactions is

$$r_i = k_i P_{C_3H_6} P_{O_2}$$

The partial pressure of propylene and oxygen was calculated using the ideal gas law. The molar and volumetric flow rates were taken from stream 5.

$$P_{C_3H_6} = \frac{\dot{n}_{C_3H_6} RT}{\dot{V}} = \frac{(1987.06 \text{ mol/min})(8.314 \times 10^{-2} \text{ L} \cdot \text{bar/K} \cdot \text{mol})(473 \text{ K})}{233358 \text{ L/min}}$$

$$= 0.335 \text{ bar } C_3H_6$$

$$P_{O_2} = \frac{\dot{n}_{O_2} RT}{\dot{V}} = \frac{(4498.68 \text{ mol/min})(8.314 \times 10^{-2} \text{ L} \cdot \text{bar/K} \cdot \text{mol})(473 \text{ K})}{233358 \text{ L/min}}$$

$$= 0.758 \text{ bar } O_2$$

The selectivities of each product were used to find the rate constants of each reaction.

$$S_{acrylic} = \frac{k_1 P_{C_3H_6} P_{O_2}}{r_{T_i}} \rightarrow k_1 = \frac{S_{acrylic} r_{T_i}}{P_{C_3H_6} P_{O_2}}$$

$$S_{acetic} = \frac{k_2 P_{C_3H_6} P_{O_2}}{r_{T_i}} \rightarrow k_2 = \frac{S_{acetic} r_{T_i}}{P_{C_3H_6} P_{O_2}}$$

$$S_{CO_2} = \frac{(k_2 + 3k_3) P_{C_3H_6} P_{O_2}}{r_{T_i}} \rightarrow k_3 = \left(\frac{1}{3}\right) \left(\frac{S_{CO_2} r_{T_i}}{P_{C_3H_6} P_{O_2}} - k_2 \right)$$

Below is a sample calculation of the rate constants at 200°C. The same calculations were performed for the rate constants at 250°C and 300°C.

$$k_1 = \frac{S_{acrylic} r_{T_i}}{P_{C_3H_6} P_{O_2}} = \frac{(0.856) (1.44 \text{ mol } C_3 / h \cdot \text{kg} - \text{cat})}{(0.758 \text{ bar})(0.335 \text{ bar})} = 174.753$$

$$k_2 = \frac{S_{acetic} r_{T_i}}{P_{C_3H_6} P_{O_2}} = \frac{(0.064) (1.44 \text{ mol } C_3 / h \cdot \text{kg} - \text{cat})}{(0.758 \text{ bar})(0.335 \text{ bar})} = 13.065$$

$$k_3 = \left(\frac{1}{3}\right) \left(\frac{S_{CO_2} r_{T_i}}{P_{C_3H_6} P_{O_2}} - k_2 \right) = \left(\frac{1}{3}\right) \left(\frac{(0.08) (1.44 \text{ mol } C_3 / h \cdot \text{kg} - \text{cat})}{(0.758 \text{ bar})(0.335 \text{ bar})} - 13.065 \right) = 1.088$$

All nine values were then used to estimate k_0 and E_a using the Arrhenius equation and plots of $\ln(k_i)$ vs $1/T$. Values were plotted in Excel for all three reactions. The slopes and intercepts of the trendlines were used to get k_0 and E_a .

$$k_0 = e^b$$

$$E_a = -mR$$

where m is the slope of the trendline, and b is the y-intercept of the trendline.

Below is a sample calculation of k_0 and E_a for the first reaction.

$$k_0 = e^{1.2214} = 88.027$$

$$E_a = -(-1144.7)(8.314) = 9.544 \frac{kJ}{mol}$$

The values of k_0 and E_a for all of the reactions are in Table I in the Process Description.

12 APPENDIX C – HEAT INTEGRATION

12.1 PROCESS UNITS AVAILABLE FOR HEAT INTEGRATION

Stream	Units	T _{in} (K)	T _{out} (K)	M (kmol/s)	C _p (kJ/kmol.K)	C (kJ/s.K)
Hot	R-100	2307	403	0.341	35.86	12.23
Hot	E-100	337	308	0.001	121.06	0.14
Hot	E-101	362	308	0.023	133.91	3.06
Cold	T-100	362	573.32	0.17	133.89	22.76
Cold	T-101	337	546.15	0.109	121.04	13.19

12.2 HEAT DUTIES OF EACH TEMPERATURE INTERVALS

Temperature Interval					
T _{hi} (K)	T _{ho} (K)	F _{sum} (kJ/s.K)	ΔH (kW)	Q (kW)	Q shifted (kW)
				0	-15772
2297	573	12.23	21085	21085	5313
573	546	-10.53	-284	20800	5028
546	393	-23.72	-3630	17170	1399
393	362	-35.95	-1115	16056	284
362	352	-13.19	-132	15924	152
352	337	-10.14	-152	15802	31
337	327	3.06	31	15772	0
327	298	3.19	93	15895	123