

Viability of the Chemical Approach to Produce Benzyl Acetate Using Zeolite Catalyst

Phase III Report

Team 12

Name	Signature	Contribution
Michael Gustafson	<i>Michael E. Gustafson</i>	20%
Bryent Lee	<i>Bryent K. Lee</i>	20%
Renee Mallick	<i>Renee Mallick</i>	20%
Emily Milburn	<i>Emily A. Milburn</i>	20%
Guilherme M. Pinto	<i>Guilherme M. Pinto</i>	20%

Table of Contents

Executive Summary	3
Introduction	4
Process	6
Process Flow Diagram	6
Process Description	7
Energy Balances & Utilities	16
Equipment List and Unit Descriptions	22
Equipment Cost Summary	29
Fixed-Capital Investment Summary	30
Safety and Environmental	31
Operating Cost and Economic Analysis	37
Conclusions and Recommendations	48
Process Flow Diagram and Material Balances	50
References	56
Appendices	58
Appendix A: Kinetics/Transport Calculations	58
Appendix B: Ternary Phase Diagrams	64
Appendix C: Energy/Utility Sample Calculations	66
Appendix D: Heat Integration	71
Appendix E: Unit Sizing and Capital Cost Sample Calculations	79
Appendix F: Distillation Start-Up Sample Calculations	94
Appendix G: Additional Capital Costs	96

EXECUTIVE SUMMARY

The purpose of this report is to optimize the production of benzyl acetate by esterification of acetic acid with benzyl alcohol over a zeolite catalyst. This report determines the economic viability of the process based on the theoretical sales price of benzyl acetate required to achieve an IRR of 15%, which we determined to be \$5.10/kg. This value is twenty percent lower than the currently supplied benzyl acetate price of \$6.40/kg. In fact, based on a full profitability analysis, it is estimated to save \$10.4 million over the course of the twenty-year expected life of the plant. Therefore, we recommend proceeding with the implantation of the benzyl acetate production plant.

The analysis is based on a desired annual production rate of 100,000 gallons of benzyl acetate at 99% purity using an assumed 6,000 operating hours per year. To meet these production requirements, reactor feeds of benzyl alcohol and acetic acid are combined in a 4:1 molar ratio. Each batch is sent to an isothermal batch reactor to achieve an acetic acid conversion of 94%. The reaction produces water as a byproduct of the main reaction and dibenzyl ether as a product of an undesired side reaction. A benzyl acetate selectivity of 95% is achieved at the reactor conditions. Separation of benzyl acetate from unused reactants and undesired products is completed using three consecutive distillation columns.

The total capital investment required for this project is \$3.5 million, and the total annual operating cost is \$1.7 million assuming only one additional operator is required for this process. This report discusses sizing and costing of all major capital equipment and the mass and energy balances for each required unit operation. It also performs detailed analysis of the major safety and environmental concerns associated with this design. While there are anticipated hazards, they were not extensive enough to affect the decision to move forward with the construction of the plant.

Before implementation, we recommend obtaining quotes from vendors on the major equipment costs required for the process, particularly the reactor and second distillation column. While it would require substantial deviations from the estimated costs to alter the decision to move forward with the plant, we recommend obtaining these quotes to reduce the risk of investment. Additionally, we recommend further investigating whether the proposed design is realistic within the facility limits and that its arrangement is advantageous in relation to the current process. Overall, the decision to proceed with the construction of the plant is based on the economic opportunity it presents and the low safety risks associated with its implementation.

INTRODUCTION

The main objective of this report is to optimize a chemical process that produces 100,000 gallons of benzyl acetate (BAC) per year and to assess its profitability. Benzyl acetate is produced for perfumery, food flavorings, soap, and other various chemical applications. In our specific case, benzyl acetate will be used as a precursor for agricultural crop protections such as insecticide and fungicide. Several methods exist to produce benzyl acetate, each requiring different feedstocks, unit operations, and catalysts. Some of these methods include (1) the esterification of acetic acid with benzyl alcohol over HZSM-5 zeolite catalyst, (2) transesterification of benzyl alcohol with vinyl acetate over immobilized lipase, (3) acetoxylation of toluene with acetic acid over PdSb/TiO₂ catalyst, (4) esterification of benzyl alcohol with acetic acid over immobilized lipase, and (5) extraction from the jasmine flower.

Between the two chemical routes (Routes 1 and 3), we found Route 1 to be a more desirable route. This decision is primarily due to Route 1 having an acetic acid conversion of 94% compared to Route 3, which has a toluene conversion of only 68%.¹ Similarly, Route 1 achieves a selectivity of 95% of benzyl acetate over its side product, dibenzyl ether (DBE), while Route 3 only achieves a selectivity of 85% over its side product, benzaldehyde.¹ Both the lower conversion and selectivity of the toluene route likely leads to more difficulty in the separation phase, making Route 3 a less desirable choice. While Route 3 has been shown to achieve conversions up to 75% and selectivities up to 100%, the conditions required to achieve these levels assume an operating pressure of 6 bar, which is likely to incur both higher operating and capital costs.² Although the profit upper bound (PUB) of Route 3 is \$2.2 million/year and the PUB of Route 1 is \$1.8 million/year, the difficulties associated with Route 3 make it less desirable overall.

After comparing the two enzymatic routes (Routes 2 and 4), we found Route 2 can achieve a conversion of 99%, while Route 4 can only achieve a conversion of 39% at the same operating conditions. Based on a smaller scale experiment for Route 4, the enzyme starts to decrease its efficiency after five full cycles.³ Results from this experiment showed a 12% decrease in conversion after utilizing the same enzyme load for 5 cycles.³ This condition, in addition to the already low conversion rate, will result in an extremely inefficient pathway that is difficult to remedy by the designed process flow. Furthermore, the PUBs for Route 2 and Route 4 are relatively similar, \$1.7 million/year and \$1.8 million/year, respectively. Thus, Route 2 was found to be more desirable.

The last method considered to produce benzyl acetate, Route 5, is highly undesirable due to its high process complexity, negative PUB, and low extraction yield of 1.9% on a flower weight basis. For these reasons, it was not examined further in this report.

After comparing the more desirable chemical and enzymatic routes (Routes 1 and 2), we decided to further examine Route 1 in this report. The decision to choose this route was primarily based on it being a safer process than Route 2, which produces acetaldehyde as a byproduct. Acetaldehyde has a flash point of -37°C, which is a storage concern.⁴ Similarly, vinyl acetate has a low flash point of -7°C and can polymerize upon exposure to light, requiring the feedstock to be stored in an enclosed container with a hydroquinone inhibitor.⁵ Additionally, acetaldehyde and vinyl acetate are possible carcinogens, so high precautions must be made to avoid worker exposure (TLV-TWA of acetaldehyde is 25 ppm, and TLV-TWA of vinyl acetate is 10 ppm).^{4,5} Selling

acetaldehyde is undesirable because of its low price and strict transportation requirements. Specifically, transportation of acetaldehyde requires refrigerated tank cars to mitigate the risks of explosions and environmental contamination.⁴ In addition to the increased safety risks, the cost of the immobilized lipase for Route 2 is about 20 times more expensive than the zeolite used in Route 1. These economic and safety concerns make Route 1 a more desirable approach.

It is important to be aware of the potential safety and environmental risks that exist for the process being proposed, Route 1. The feedstocks and products of the process are all toxic chemicals; therefore, safety precautions need to be taken to avoid direct contact with operators. Most compounds used in this process have a low TLV-TWA of 10 ppm, posing serious risks to the operators if these chemicals are released within the facility for an extended period of time.^{6,7,8,9} Due to the corrosiveness of acetic acid, equipment needs to be made of stainless steel to prevent corrosion and degradation.⁶ All the chemicals have very high auto ignition temperatures but moderate flash points and flammability ranges. Due to these low flammability ranges, chemicals need to be closely monitored and stored under atmospheric conditions of 25°C and 1 atm.^{6,7,8,9} Finally, storage is a critical part of the plant, requiring precise control of liquid levels and preventive measures in the case of emptying or overfilling. Intermediate storage tanks should be closely monitored, with the implementation of high-level and low-level alarms to warn operators if a volume limit is going over or below a specific threshold. All the safety hazards and preventive measures are explained in more detail in the safety section of the report.

Environmental protection is a major factor when designing a new chemical process, and this case is no exception. All the chemicals used in this process, except water, have a high level of aquatic toxicity and cannot be released into the environment.^{6,7,8,9} Benzyl alcohol and dibenzyl ether have particularly severe aquatic toxicity values of 55 mg/L and 2.2 mg/L, respectively.^{7,8} Based on the Clean Water Act (CWA) regulated by the Environmental Protection Agency (EPA), the water being produced from the reactions cannot be released into the environment.¹⁰ Therefore, all the wastewater produced by this process should be sent to wastewater treatment. All chemicals stored within the plant are listed in the Toxic Substances Control Act (TOSCA) inventory, requiring specific reporting of quantities being stored in the plant.¹¹ One benefit of this process design is that no compounds are considered hazardous air pollutants (HAPs) by the EPA.¹² Also, there is no direct production of carbon dioxide or methane other than the minimal burning of natural gas required for utilities. All the environmental hazards, preventive measures, and regulations are examined in more detail in the environmental section of the report.

PROCESS FLOW DIAGRAM

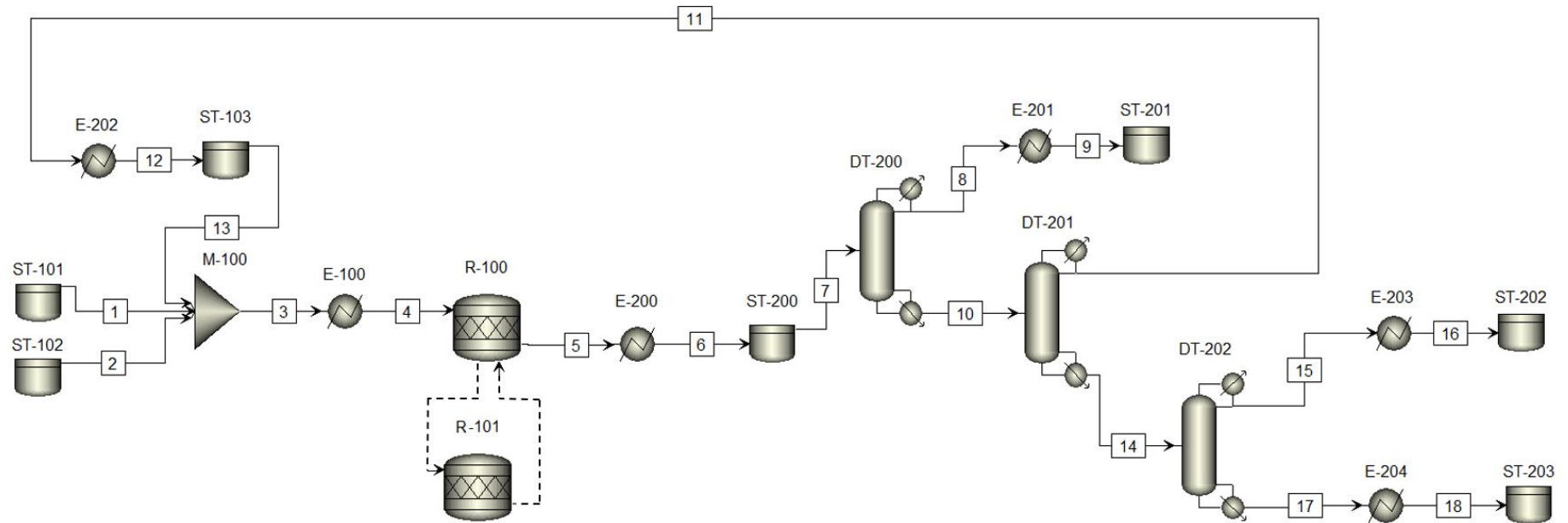


Figure 1. Process Flow Diagram (P-100 not shown but used to load/unload R-100)

PROCESS DESCRIPTION

Assumptions

The process being presented was modeled in Aspen Plus using the NRTL-HOC thermodynamic package. The initial masses of the two reactants, benzyl alcohol and acetic acid, were estimated for a desired annual production of 100,000 gallons of benzyl acetate by assuming 5 continuous days in a work week and 50 work weeks in an operating year. Scaled to a weekly basis, this assumption results in a desired benzyl acetate production of 7,980 kg per week. This weekly amount was then used to calculate the number of batches required per week and the amount of benzyl acetate needed to be produced in each batch.

Originally, the base case found that 36 batches could be run each week with each batch producing 222 kg of benzyl acetate. For this calculation, we assumed six hours each week for start-up, six hours each week for shutdown, three hours per batch, and forty minutes for catalyst regeneration every six batches. The last assumption is based on the zeolite catalyst, Micro/Meso-HZSM-5, being viable for six batches before regeneration is required.

However, new assumptions were used to achieve a more realistic schedule for weekly production. Each week, we now assume eight hours for start-up and eight hours for shutdown, meaning only 104 hours are available for operation per week (5,200 hours per year). Additionally, we now assume each catalyst regeneration cycle requires 12.7 hours: six hours for unloading catalyst from the reactor, forty minutes for the catalyst regeneration, and six hours for loading catalyst back into the reactor along with any intermediate reactor cleaning. Catalyst regeneration is still planned to occur every six batches. Lastly, we still assume each batch requires three hours: thirty minutes for loading reactants, two hours for the reaction, and thirty minutes for unloading the resulting product mixture. Using these assumptions, a Gantt chart was created to better visualize the number of batches required per week, as shown by Figure 2.

Based on the new assumptions, we determined that 18 batches could be run each week with each batch producing 444 kg of benzyl acetate. Overall, this schedule allots 54 hours per week for the batch reaction and 86 hours per week for continuous separations. Additionally, a total of 4.5 hours of series start-up time is required for the distillation towers. Figure 3 shows a close-up of the first six batches and regeneration cycle of each week for clarity.

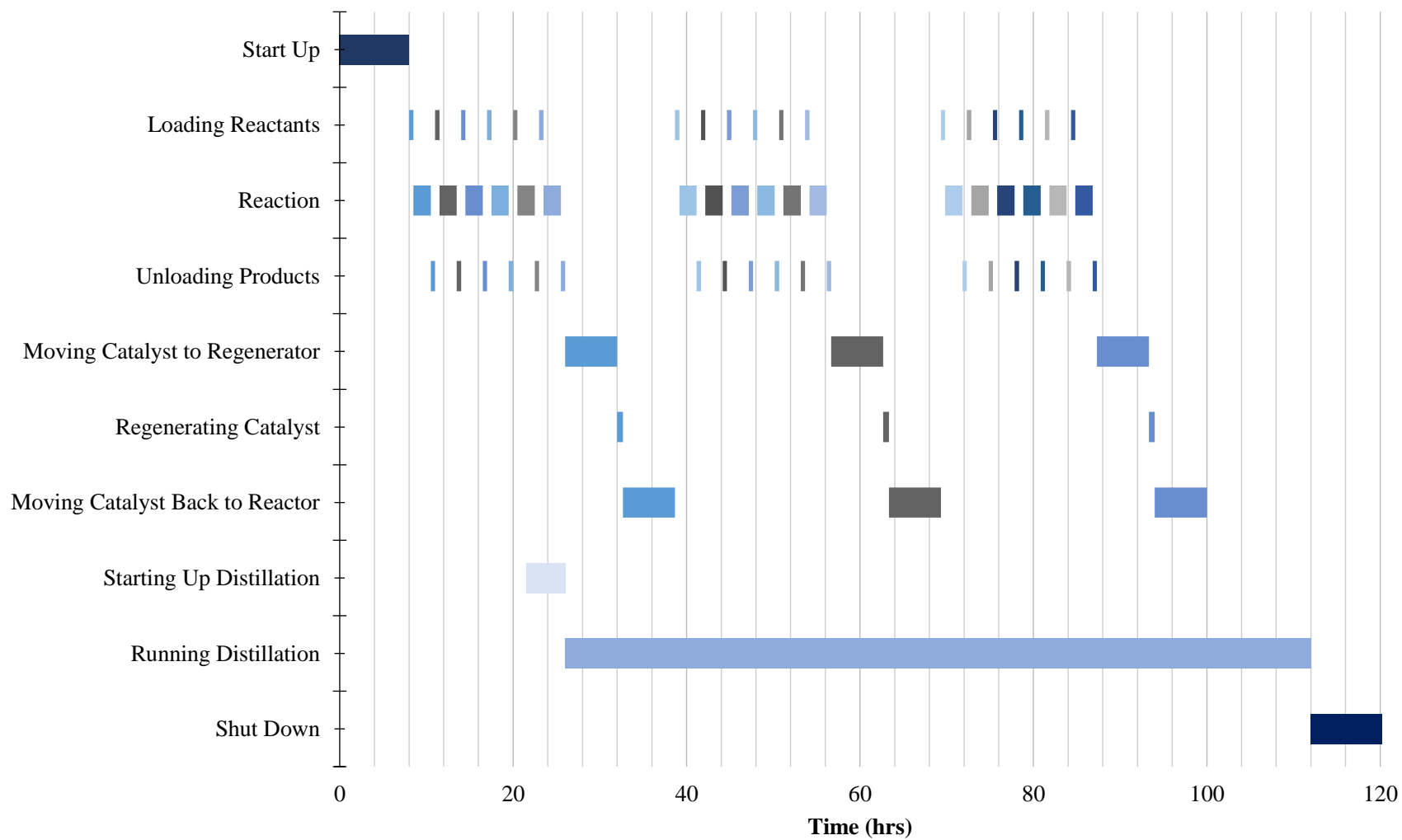


Figure 2. Weekly Gantt Chart

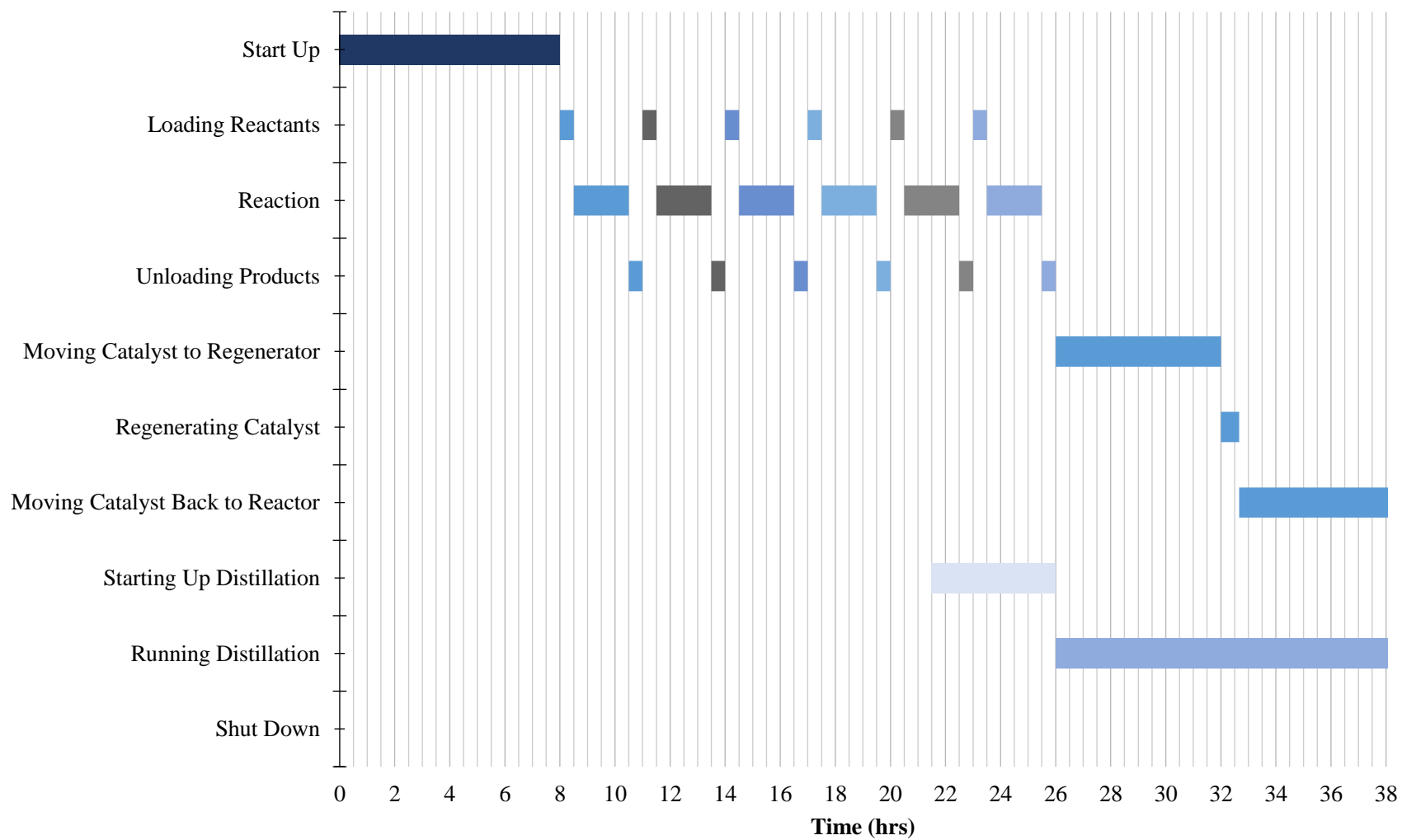


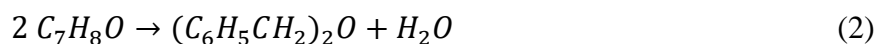
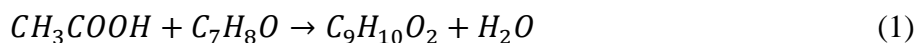
Figure 3. First Six Batches and Regeneration Cycle in the Weekly Gantt Chart

Inlet Conditions

The initial batch amounts of 1360 kg benzyl alcohol and 189 kg acetic acid are fed into the system each week at standard conditions (25°C and 1 atm) from storage totes (ST-101 and ST-102, respectively), which are 275-gallon containers. The reactants are combined at M-100 prior to entering the reactor (R-100). After the initial six batches, M-100 will combine unused reactants with fresh feed for the remainder of the week. The unused reactants, consisting of benzyl alcohol (98.7% by mass) and a small amount of acetic acid, are held in a storage tank (ST-103). For each batch, M-100 will pull 1018 kg (1007 kg benzyl alcohol and 11 kg acetic acid) from ST-103 first and then fill the remaining required mass with fresh feed from ST-101 and ST-102.

Reactor: R-100

For the batch process, Microsoft Excel (2019) was used to model an isothermal jacketed batch reactor with the following reactions occurring in a slurry.



The kinetics of this reaction were assumed to match the kinetic data for the esterification of acetic acid with benzyl alcohol over Micro/Meso-HZSM-5 presented in Nandiwale et al.¹³ Therefore, the reaction was assumed to follow this first-order kinetic equation:

$$r = Ae^{-E_a/RT}[CH_3COOH] \quad (3)$$

where benzyl alcohol is fed in excess, $E_a = 15.07$ kJ/mol, and $A = 2.34$ min⁻¹ based on a catalyst loading of 10% (wt.% of acetic acid). With the given operating temperature of 393 K, the reaction rate constant is 0.023 min⁻¹. Additionally, this operating temperature, catalyst loading, and molar feed ratio were known to achieve a 94% conversion of acetic acid and a 95% selectivity of benzyl acetate over dibenzyl ether, which were both verified in our kinetic calculations. It is important to note that other temperatures were considered, but the rate of increase in acetic acid conversion diminishes after 393 K, as shown in Figure 4. While it is possible to increase the temperature to achieve an acetic acid conversion of 100%, the selectivity of benzyl acetate over dibenzyl ether lowers from 95% to less than 83%.¹² Therefore, 393 K was determined to be an appropriate reactor condition. Additionally, both this temperature and the decision to run 18 batches per week resulted in a catalyst loading of 19 kg per batch.

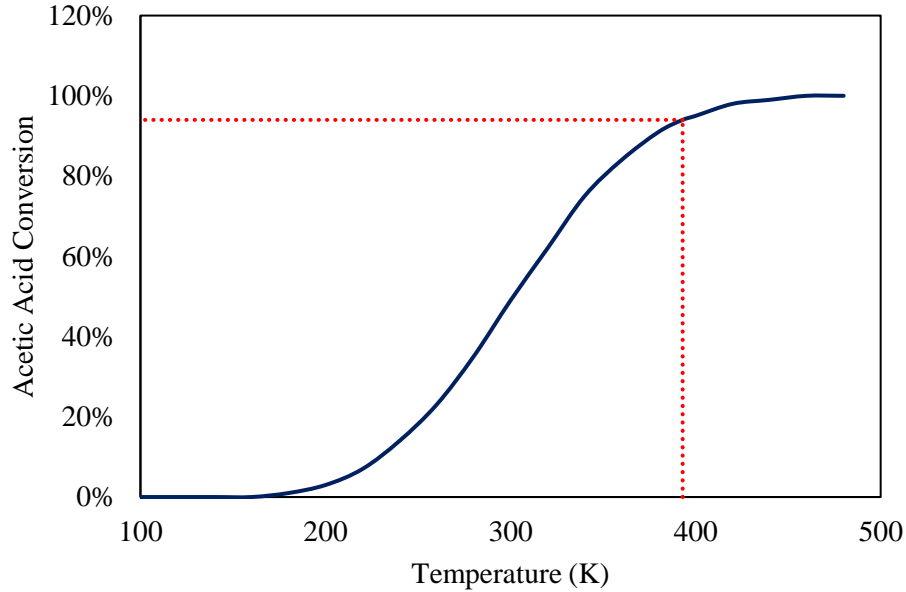


Figure 4. Conversion Achieved in Two Hours at Various Temperatures

The above kinetic parameters are assumed to include pore mass resistance within the zeolite. Additionally, external resistance surrounding the zeolite beads is negligible when applying a stirring rate of 200 rpm within the reactor using a Rushton stirrer.¹⁴ This agitation results in a Damköhler number (Da) less than 0.1, which suggests that the conversion of acetic acid is kinetics-limited. The dimensionless Damköhler number is calculated to be 0.0491 using the formula shown below in Equation 4:

$$Da = \frac{-r_A}{k_L * a * [C_A]_{bulk}} \quad (4)$$

where $-r_A$ is the maximum reaction rate per reactor volume, k_L is the mass transfer coefficient equal to 0.15 cm/s, a is the total particle surface area per reactor volume and $[C_A]_{bulk}$ is the concentration of the limiting substrate (acetic acid) in the bulk.¹⁵ Detailed calculations for the Damköhler number are shown in Appendix A-3. We concluded that if the particle size is greater than 1.5 microns, the Damköhler number will be less than 0.1 at a stirring rate of 200 rpm. The zeolite was found to have a particle size of approximately 45 microns, which fits well within this requirement.¹⁶

Each week, the reactor runs 18 batches with each batch producing 444 kg of benzyl acetate. As previously mentioned, 1360 kg (12.6 mol) of benzyl alcohol and 189 kg (3.15 mol) of acetic acid are required for each batch. Benzyl alcohol must be fed in excess (4:1 molar ratio with acetic acid) in order to assume a first-order reaction.

Lastly, the reactions occurring within the reactor are endothermic, so 168,000 kJ/batch of heating is required to maintain the reactor temperature at 393K (120°C). Based on heat of reaction, 5,557 kg/batch of hot oil is required to maintain isothermal conditions, as calculated in Appendix C-1.

Catalyst Regeneration Unit: R-101

The catalyst used in the reaction, Micro/Meso-HZSM-5, is viable for one fresh run and five recycles, totaling six cycles before regeneration is required.¹³ Due to this fast catalyst deactivation, regeneration is extremely important to restore catalyst activity and benzyl acetate selectivity. The main cause of deactivation of Micro/Meso-HZSM-5 catalyst is coke deposition within the channels of the zeolite. The coke can be removed by means of combustion while increasing temperatures from 350°C to 550°C at a rate of 5°C per minute.¹⁷

As noted in the assumptions, each catalyst regeneration cycle requires 12.7 hours: six hours for unloading catalyst from the reactor, forty minutes for the catalyst regeneration, and six hours for loading catalyst back into the reactor along with any necessary reactor cleaning. Catalyst regeneration is planned to occur every six batches.

Distillation Columns: DT-200, DT-201 & DT-202

The first distillation column (DT-200) is fed by a storage tank (ST-200), which is filled with products and unused reactants. DT-200, operating at 1 atm, separates water from the unused reactants and other products. In the base case, DT-200 requires 13 stages and a reflux ratio of 1. However, since the number of batches per week decreased from 36 to 18 batches, the size of each batch increased. Therefore, a higher flowrate is sent from ST-200 to DT-200. By using a DSTWU column, the minimum number of stages and minimum reflux ratio were found to be 4 and 0.2, respectively. These values were plugged into a RadFrac column as initial values and varied until a purity of 96% by mass of water was achieved in the distillate. The result is that DT-200 requires 12 stages and a reflux ratio of 1, which is slightly smaller than the base case. The molar distillate to feed ratio used was 0.198. The distillate stream is cooled to 25°C and stored in ST-201, which is then sent to wastewater treatment for neutralization and removal of remaining amounts of benzyl alcohol and acetic acid. While we considered optimizing DT-200 to produce a “white vinegar” internal cleaner as the distillate stream, the amount of benzyl alcohol in the stream could not be lowered below the maximum allowed mass fraction of 0.1%.

A flash unit was considered to replace DT-200; however, a purity of 96% by mass for water could not be obtained due to water’s binary interaction with acetic acid. Liquid-liquid extraction was also considered over a distillation column. However, due to the extra complexity and capital cost associated with liquid-liquid extraction, we do not recommend it.

The bottoms of DT-200 are then fed into the second distillation column (DT-201), which also operates at 1 atm. DT-201 separates the unused reactants from benzyl acetate and dibenzyl ether. The unused reactants are primarily composed of benzyl alcohol since it is fed in excess to the reactor. This separation proved to be the most challenging since the boiling points between benzyl alcohol and benzyl acetate only differ by 11°C. In the base case, DT-201 requires 99 stages and a reflux ratio of 11. Again, a DSTWU column was used to find the minimum number of stages and minimum reflux ratio, which were 47 and 9, respectively. These values were plugged into a RadFrac column and varied until the distillate reached its peak purity of 98.6% by mass for benzyl alcohol due to the remaining unreacted acetic acid. To achieve this purity, DT-201 requires 94

stages and a reflux ratio of 9.5. Additionally, these operating conditions allowed for the final benzyl acetate product to achieve 99% by mass purity. The molar distillate to feed ratio used was 0.753. The distillate stream is ultimately cooled to 25°C and stored in ST-103 for use as recycled reactants.

Further optimization of the number of stages and reflux ratio were considered as the mass purity of benzyl acetate could be as low as 96%, with 4% benzyl alcohol. While the lower mass specification purity for benzyl acetate product allowed DT-201 to reduce the number of stages to 81 and the reflux ratio down to 8, the distillate purity dropped to 98% benzyl alcohol by mass. Due to the additional benzyl acetate in the recycle, a non-negligible amount of valuable product would be sent back to the reactor. To avoid these recycling issues, 94 stages and a reflux ratio of 9.5 were used for DT-201, which results in a distillate purity of 98.6% of benzyl alcohol and product purity of 99.4% for benzyl acetate.

The remaining products of benzyl acetate and dibenzyl ether from the bottoms of DT-201 are sent to a third and final distillation column (DT-202) to be separated at 1 atm. In the base case, 10 stages and a reflux ratio of 0.6 were required for the desired product purities of 99% by mass. A DSTWU column found that a minimum of 5 stages and reflux ratio of 0.2 were required initially. In order to achieve purities of 99% by mass for both products, these DSTWU estimation values were varied. In the RadFrac column, 10 stages and a reflux ratio of 0.4 were required for the desired purities. The molar distillate to feed ratio used was 0.95. The distillate, mainly benzyl acetate, is then cooled to 25°C and stored in ST-202. Similarly, the bottoms, mainly dibenzyl ether, is cooled to 25°C and stored in ST-203.

Heaters & Coolers

Heat exchanger units were used to change temperatures around several different process units. E-100 is used to pre-heat the mixed feeds stream to the reactor temperature of 120°C, while E-200 cools the reactor outlet stream to 25°C in order to be stored in ST-200 safely. Both E-100 and E-200 are considered batch since they occur before and after the reactor. The remaining heat exchanger units are considered continuous since they are in the separations section. E-201 cools the wastewater stream exiting DT-200 before storing it in ST-201 and sending it to wastewater treatment. E-202 cools the recycled unused reactants to 25°C before storing them in ST-103, so they can be properly mixed with the necessary fresh feeds at the same temperature. E-203 and E-204 cool the product streams exiting DT-202 to a desired product temperature of 25°C before storing each product in its respective storage tank (ST-202 and ST-203).

Storage Tanks

The reactants, benzyl alcohol and acetic acid, are introduced to the system from ST-101 and ST-102, which are simply storage totes. The reactants are purchased in 275-gallon totes every two weeks, and they are used directly to feed each batch reaction using specialty tote-to-process pumps.¹⁸

ST-200 and ST-103 are considered intermediate tanks because they are constantly being filled and drained during the process. ST-200 holds the reactor outlet before feeding the continuous separation, while ST-103 holds the recycled unused reactants. The base case originally filled ST-200 with three batches before continuous separation began. However, after further analysis, it was found that filling ST-200 with only three batches resulted in the storage tank being drained before separations were completed. Therefore, a full inventory analysis was completed to ensure the distillation columns did not run dry for storage tanks ST-200 and ST-103, as shown by Figures 5 and 6.

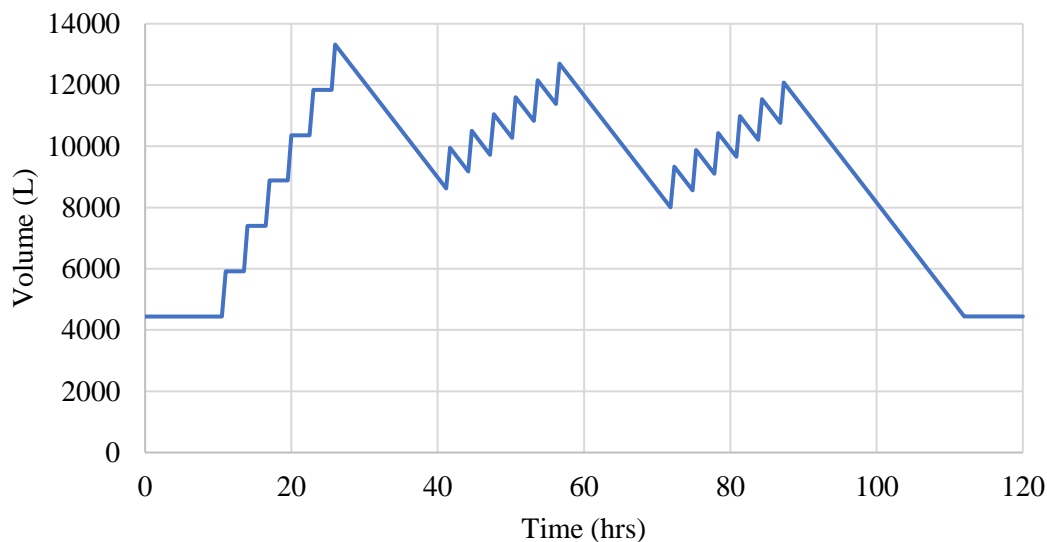


Figure 5. ST-200 Weekly Inventory Chart.

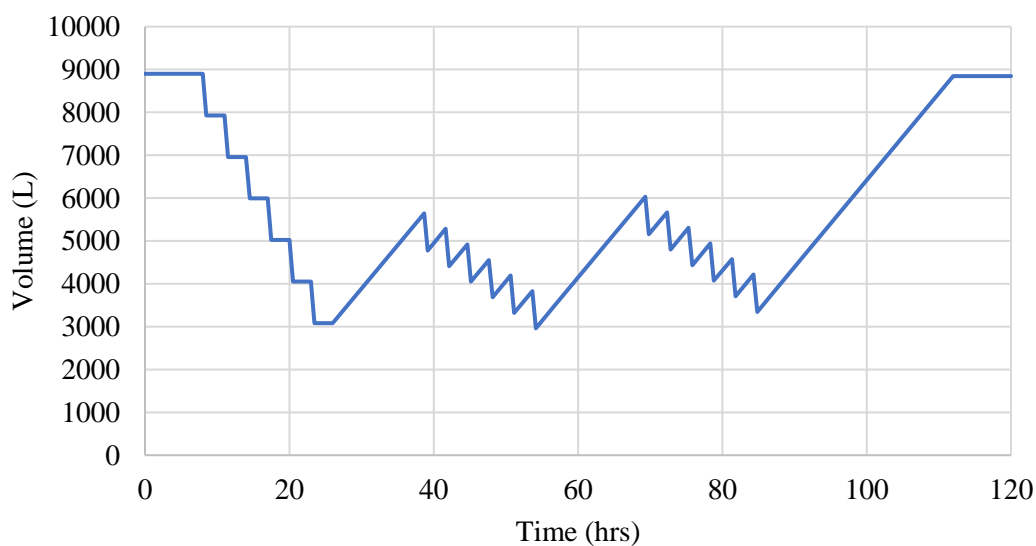


Figure 6. ST-103 Weekly Inventory Chart.

We determined that six batches were required to fill ST-200 before starting the continuous distillation for the week; this method ensures that the tank does not run dry by the end of the week. The inventory analysis was also used to calculate the volume needed for each intermediate tank. In order to achieve a non-zero baseline level in each of the tanks, an extra three batches are run for the very first week of the year. By running these additional batches, ST-200 maintains a baseline level of 4440 L. Both the initial batches at the start of the year and the six batches at the beginning of each week, ensure the distillation columns never run dry.

All finished products are also sent to tanks for storage. Their volumes were calculated on a two-week basis. ST-201 and ST-203, which store wastewater and dibenzyl ether respectively, are then transferred to 275-gallon totes for transportation. The wastewater is transported to a treatment plant and dibenzyl ether is sold by the tote. Lastly, ST-202 stores the desired product, benzyl acetate, which is later used as a feedstock for a downstream process.

ENERGY BALANCE AND UTILITY REQUIREMENTS

The major energy requirements of the process are provided in Tables I(a)-(d) below for each unit. Table I(a) describes the energy required for each batch, whereas Tables I(b)-(d) are for continuous energy requirements.

For the batch section, the utility per batch of the reactor (R-100) was determined by calculating the heat of reaction for two hours. To find the maximum rate for the reactor, the initial rate of acetic acid conversion was used. The utility per batch of the catalyst regeneration unit (R-101) was determined by calculating the rate of heat transfer from hot air to the catalyst assuming 40 minutes per regeneration. To find the maximum rate for the regeneration unit, the heat capacity based on the maximum temperature was used. The heat exchangers were assumed to operate for three hours per batch. However, the reactor pump (P-100) was assumed to operate for one hour per batch, the time required for loading and unloading. Lastly, the agitator was assumed to operate only during the two hours required for the reaction per batch. The calculations for the batch energy requirements can be found in Appendix C-3.

For the continuous energy requirements, Figures 7-9 are provided below to better understand the breakdown between required energy for each unit under the designated areas of heating, cooling, and electricity. The total energy required for heating is 2,280,000 kJ/hr, which costs \$46,000/yr. As shown in Figure 7, the reboiler in DT-201 requires the most energy because it is the largest tower due to the challenging separation of benzyl alcohol and benzyl acetate. The total energy required for cooling is 2,170,000 kJ/hr, which costs \$49,000/yr. As shown in Figure 8, the largest cooling requirement is from the condenser in the second distillation column, DT-201. Again, it makes sense that DT-201 requires the most cooling because it handles the difficult separation of benzyl alcohol and benzyl acetate. As shown in Figure 9, the catalyst regeneration unit requires the most electricity for operation, which makes sense because it is heating the catalyst to temperatures as high as 550°C using an electric coil. Hot oil could not be used for the regeneration unit because its maximum temperature is 340°C, which is well below the required 350°C-550°C temperature ramping range. The total energy required for electricity is 15,500 kJ/hr, which costs \$800/yr. Overall, the process requires similar amounts of heating and cooling, which are extraordinarily greater than the electricity requirement.

Table I(a). Data displaying the energy requirements for all units running on a batch basis

Unit		E-100	P-100	R-100	R-100 Agitator	E-200	R-101
Quantity		Heating	Pressurizing	Heating	Stirring	Cooling	Heating
Utility over a batch	kJ/batch	3.00×10^5	3.35×10^3	1.68×10^5	1.07×10^3	-3.75×10^5	7.71×10^3
Maximum rate	kW	27.8	0.932	576.1	0.148	27.8	3.27
Min. Temp. of Batch Material	Centigrade	-	-	-	-	25	350
Max. Temp. of Batch Material	Centigrade	120	120	120	120	-	550

Table I(b). Data displaying the energy requirements and functional state change for heat exchangers

Unit		E-100	E-200	E-201	E-202	E-203	E-204
Operation		Heating	Cooling	Cooling	Cooling	Cooling	Cooling
Heat Duty	kJ/hr	1.00×10^5	-1.25×10^5	-5.86×10^3	-1.26×10^5	-5.17×10^4	-5.21×10^3
Net Work	kJ/hr	-	-	-	-	-	-
ΔT	$^{\circ}\text{C}$	94.8	-94.9	-75.1	-170	-189	-262
ΔP	kPa	-	-	-	-	-	-
Phase Change		-	-	-	-	-	-
Utility Required		Hot Silicon Oil	Chilled Water	Chilled Water	Chilled Water	Chilled Water	Chilled Water
Utility Costs	\$/yr	\$1,200	\$1,700	\$100	\$2,900	\$1,200	\$100
Oil Flow Rates	kg/hr	179					
Chilled Water Flow	tons	-	9.86	0.463	9.93	4.08	0.412

Table I(c). Data displaying the energy requirements and functional state change for the reactor, pump, agitator, and catalyst regeneration unit

Unit		R-100 Pump	R-100	R-100 Agitator	R-101
Operation		Pressurizing	Heating	Stirring (200 rpm)	Heating
Heat Duty	kJ/hr	-	4.21×10^4	-	-
Net Work	kJ/hr	3.35×10^3	-	5.33×10^2	1.16×10^4
ΔT	$^{\circ}\text{C}$	-	-	-	200
ΔP	kPa	37.9	-	-	-
Phase Change		-	-	-	-
Utility Required		Electricity	Hot Silicon Oil	Electricity	Electricity
Utility Costs	\$/yr	\$200	\$1,000	\$30	\$600
Oil Flow Rates	kg/hr	-	2778	-	-
Chilled Water Flow	tons	-	-	-	-

Table I(d). Data displaying the energy requirements and functional state change for the distillation columns

Unit		DT-200	DT-200	DT-201	DT-201	DT-202	DT-202
Operation		Condensation	Boiling	Condensation	Boiling	Condensation	Boiling
Heat Duty	kJ/hr	-4.26×10^4	1.67×10^5	-9.73×10^5	9.68×10^5	-3.57×10^4	3.62×10^4
Net Work	kJ/hr	-	-	-	-	-	-
ΔT	$^{\circ}\text{C}$	-	-	-	-	-	-
Operating Temp	$^{\circ}\text{C}$	100	200	195	216	214	287
ΔP	kPa	-	-	-	-	-	-
Phase Change		Vapor to Liquid	Liquid to Vapor	Vapor to Liquid	Liquid to Vapor	Vapor to Liquid	Liquid to Vapor
Utility Required		Chilled Water	Hot Silicon Oil	Chilled Water	Hot Silicon Oil	Chilled Water	Hot Silicon Oil
Utility Costs	\$/yr	\$2,000	\$6,900	\$39,300	\$35,300	\$1,900	\$1,700
Oil Flow Rates	kg/hr	-	894	-	5606	-	640
Chilled Water Flow	tons	6.72	-	134	-	6.33	-

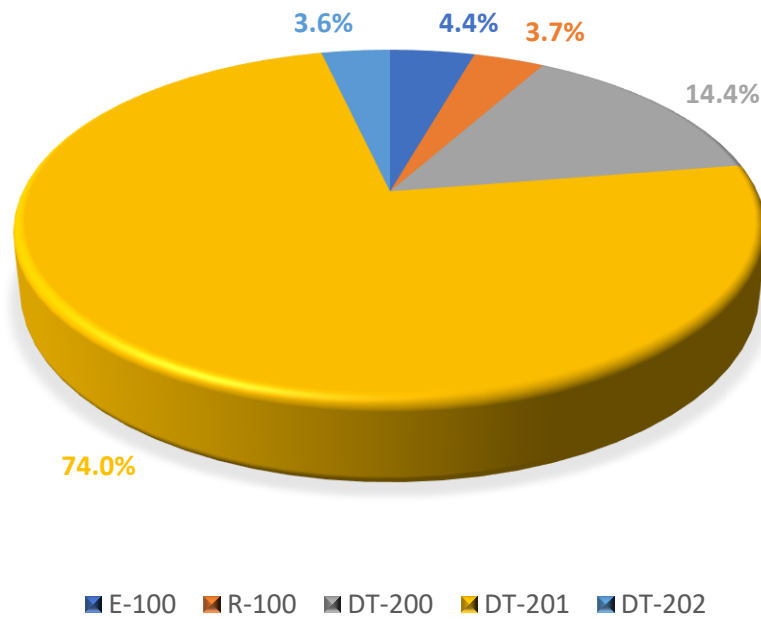


Figure 7. Percentage distribution of energy for heating required by specific units

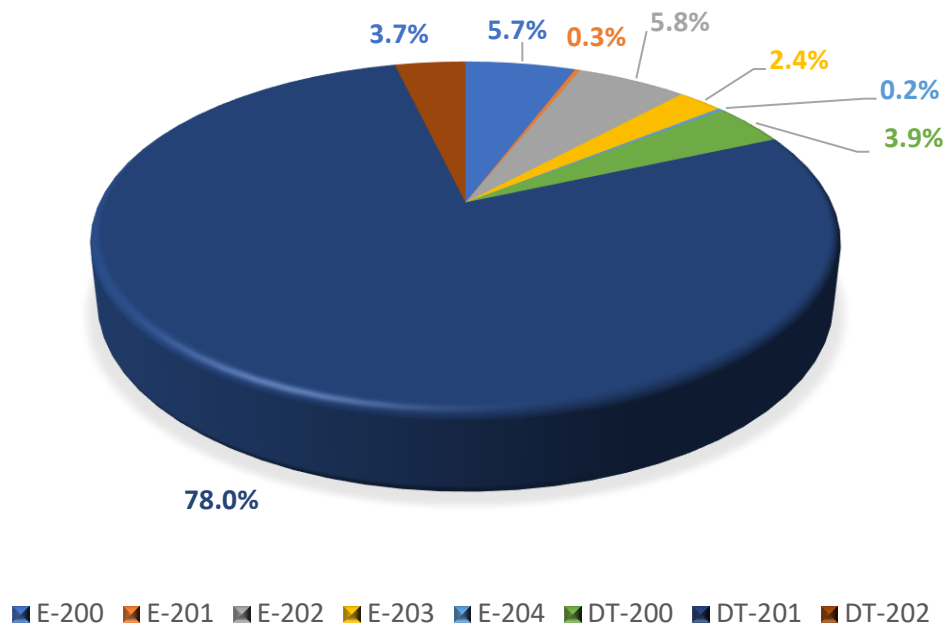


Figure 8. Percentage distribution of energy for cooling required by specific units

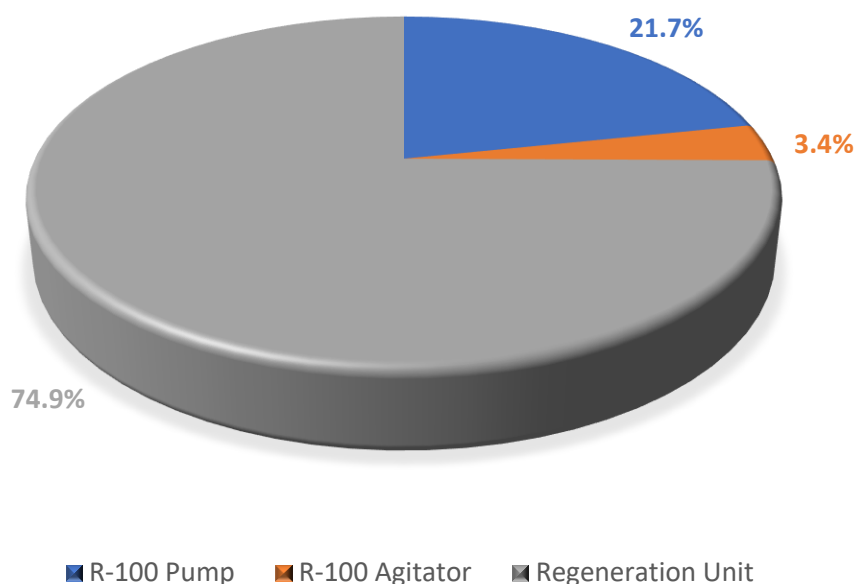


Figure 9. Percentage distribution of energy for electricity required by specific units

A hot oil recirculation system was installed for required heating of specific units. The hot oil selected was Shell Thermia B because it fit the heating requirements and maintained a minimum driving temperature difference of 10°C for every unit.²⁴ The maximum temperature of 340°C for Shell Thermia B exceeded the highest temperature of 287°C required by the reboiler in DT-202. The hot oil system is heated using natural gas, which was a cheaper alternative than electricity.

Heat integration was considered to reduce utility costs for heating and cooling. A full heat exchanger network was designed to explore the possibilities for heat integration. A minimum temperature difference of 10°C was maintained throughout the process, and a “cold pinch” temperature was chosen. A temperature interval diagram and cascade diagram were constructed to find the cold pinch temperature of 200°C as shown in Appendix D-1. From there, the possible unit combinations for heat integration could be selected. The three combinations that were chosen for heat integration were: (1) the reboiler of DT-200 with E-203, (2) the reboiler of DT-201 with E-204, and (3) the condenser of DT-201 with E-100.

The original heat exchanger, E-203, is broken into two new heat exchangers, E-203A and E-203B. E-203A will be placed in the original location of E-203, and E-203B will be placed directly after the reboiler in DT-200. The heat duties of these two heat exchangers can be calculated from the temperature differences and must sum to equal the original heat duty of E-203. The heat duty from E-203B is equal to our energy savings, which can be used to calculate the total energy savings found for chilled water in the heat exchanger and hot oil in the reboiler. The exact process was repeated for E-204 and the reboiler in DT-201. For E-100, the condenser in DT-201 can transfer the full amount of energy required by the heat exchanger. All calculations involved with heat integration can be found in Appendix D-2 and D-3, but a table summarizing total energy savings are displayed below in Table II.

Table II. Data displaying the distribution of energy saved from performing heat integration

	Saved Energy (kJ/hr)	Saved Utility Cost (\$/yr)
Hot Oil	102,000	\$1,300
Chilled Water	102,000	\$2,400

However, with heat integration, the capital costs of the heat exchangers increased by \$13,000. In order to determine if heat integration should be implemented, the theoretical price of benzyl acetate needed to achieve an IRR of 15% was considered. Without heat integration, the price of benzyl acetate was found to be \$5.10. With heat integration, the price of benzyl acetate was still found to be \$5.10, resulting in no effect on the price. Therefore, it is not recommended to proceed with implementing heat integration due to the increase in complexity of the process.

EQUIPMENT LIST AND UNIT DESCRIPTIONS

Reactor: R-100 (including Pump and Agitator)

The isothermal batch reactor is maintained at 120°C using a heating jacket of hot oil. Since the reactions are endothermic, 168,000 kJ/batch of heating is required to maintain the reactor temperature. The required amount of hot oil was calculated to be 5,557 kg/batch, based on the heat of reaction, specific heat capacity of Shell Thermia B, and a temperature difference of 10°C. The surface area required for the heating jacket around the reactor was found using the heat transfer equation.¹⁹

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

where Q is the heat of reaction, U is the heat transfer coefficient, A is the surface area, and ΔT_{LM} is the logarithmic mean temperature difference. The value of U was found to be 35 BTU/ft² hr °F, assuming the upper limit of a liquid-liquid media with oil tube side.¹⁹ The value of ΔT_{LM} was calculated assuming a countercurrent exchange and using both the hot oil temperature difference and constant reactor temperature. The surface area required by the heating jacket was found to be 13.5 m². The reactor volume was found to be 1.67 m³ with a diameter of 0.45 m and height of 10.5 m. The tall reactor is a direct result of the amount of surface area required to maintain the reactor temperature. Appendix E-1 shows how these values were calculated.

The slurry reactor, R-100, includes an agitator at 200 rpm and a heating jacket. An autoclave was used to cost our reactor because it is a vertical, cylindrical stirred-tank reactor. The equation chosen for the autoclave costing used a material of stainless steel. The bare module cost of \$448,000 includes a turbine agitator and heat-transfer jacket (see Appendix E-1 for calculation). The operating cost of the reactor is \$1,000/yr.

Lastly, the reactor requires a pump to load and unload the liquid reactants and products, taking 30 minutes each. The total power required is 0.93 kW, which costs \$175/yr to operate. The bare module cost is \$24,000 as shown in Appendix E-2. Because the reactor pump is a crucial item for the batch process, a spare pump is kept on site.

Catalyst Regeneration Unit: R-101

A similar approach for sizing and costing of the reactor was used for the catalyst regeneration unit. The volume of R-101 was found to be 0.026 m³ with a diameter of 0.25 m, and height of 0.53 m. These dimensions are based on 19 kg of catalyst being regenerated after every six batches. The bare module cost is \$8,600, which is based on a material of stainless steel 316 (see Appendix E-3 for calculation). Catalyst regeneration is obtained by combustion while increasing temperatures from 350°C to 550°C using an electrical coil.¹⁵ Therefore, the operating cost is \$600/yr.

Distillation Columns: DT-200, DT-201 & DT-202

Our process requires three packed-bed distillation columns: DT-200, DT-201 and DT-202. The first column (DT-200) separates out water using 12 equilibrium stages. The second column (DT-201) separates unused reactants to be recycled back to the reactor using 94 equilibrium stages. The third and final column (DT-202) separates the products, benzyl acetate and dibenzyl ether, using 10 equilibrium stages. All distillation columns are operated at 1 atm.

The diameters of the distillation columns are as follows: DT-200 = 1.20 ft, DT-201 = 2.43 ft, and DT-202 = 0.53 ft. These diameters were calculated using the total boil-up rate and flooding velocity as shown in Appendix E-4. For all three distillation columns, ceramic Raschig rings of 0.5 inches ($\$20/\text{ft}^3$) were used for packing since the tower diameters were less than 2.5 ft. The height equivalent to a theoretical plate (HETP) was calculated by multiplying 1.5 to the packing material diameter to give a value of 0.75 ft. The packing height was found by multiplying the number of equilibrium stages by the HETP. The packing height of the distillation columns are as follows: DT-200 = 9 ft, DT-201 = 70.5 ft, and DT-202 = 7.5 ft.

The bare module cost of each distillation column, including reboilers and condensers, are as follows: DT-200 = \$87,000, DT-201 = \$675,000, and DT-202 = \$50,000. All distillation columns are made using stainless steel 316 to prevent corrosion from acids. A sample calculation is shown in Appendix E-4. The operating costs for each distillation column are based on the utility costs of the reboiler and condenser. The total operating costs are: \$9,000/yr for DT-200, \$75,000/yr for DT-201, and \$4,000/yr for DT-202.

For the calculation of start-up time, the distillation columns were assumed to have trays. The number of actual trays was found using the number of equilibrium stages from ASPEN and the tray efficiency from the O'Connell Correlation.¹⁹ The total liquid hold-up in the distillation column was then calculated using the column cross-sectional area and the number of trays. The fill-up time for each distillation column was calculated using the boil-up rate and the total liquid hold-up. Multiplying the fill-up time by 5 to ensure equilibrium has been met provided us with the start-up time for each distillation column. The start-up times for DT-200, DT-201, and DT-202 are as follows: 26 minutes, 3.3 hours, and 35 minutes. The distillation columns start up in series, meaning DT-200 must start up before DT-201, and DT-201 must start up before DT-202. Therefore, the total start-up time for distillation is 4.5 hours. A sample calculation is shown in Appendix F.

Heat Exchangers: Heaters and Coolers

There are six heat exchangers throughout the process: one heater (E-100) and five coolers (E-200, E-201, E-202, E-203, E-204). The heater uses hot oil, and the coolers use chilled water. E-100 preheats the reactor feed to the desired reaction temperature of 120°C. E-200 cools the reactor outlet to 25°C before storing it in ST-200. E-201 cools the wastewater stream to 25°C before storing it in ST-201. E-202 cools the recycled unused reactants to 25°C before storing them in ST-103. E-203 cools the benzyl acetate product to 25°C before storing it in ST-202. Finally, E-204 cools the dibenzyl ether product to 25°C before storing it in ST-203.

The surface area required for heat exchange was found using the heat transfer equation:¹⁹

$$Q = UA\Delta T_{LM} \quad (6)$$

where Q is the heat duty, U is the heat transfer coefficient, A is the surface area, and ΔT_{LM} is the logarithmic mean temperature difference.

For the heater (E-100), the value of U was found to be 30 BTU/ft² hr °F.¹⁹ The ΔT_{LM} was calculated using a countercurrent exchange of the hot oil and the heater fluid. The surface area required by E-100 was found to be 11.6 ft². The associated operating cost for heating is \$1,200/yr.

For the coolers, the value of U was found to be 100 BTU/ft² hr °F.¹⁹ The ΔT_{LM} was calculated using a countercurrent exchange of the chilled water and the cooler fluid. Table III shows the surface area and associated operating cost for each cooler.

Table III. Surface Area and Operating Costs for Each Cooler

	E-200	E-201	E-202	E-203	E-204
Surface Area (ft ²)	20.0	1.10	13.5	5.15	0.41
Operating Costs per year	\$1,700	\$140	\$2,900	\$1,200	\$120

In our process, all heat exchangers have a heat exchange surface area less than 200 ft², meaning double-pipe heat exchangers were selected and costed appropriately.¹⁹ Stainless steel was chosen to prevent corrosion from acids. The bare modules costs for all heat exchanges are as follows: E-100 = \$9,800, E-200 = \$11,500, E-201 = \$7,200, E-202 = \$10,800, E-203 = \$9,200, and E-204 = \$6,200. A sample calculation is shown in Appendix E-5.

Storage Tanks

The reactants, benzyl alcohol and acetic acid, are fed to the system from ST-101 and ST-102, respectively. The reactants are purchased in 275-gallon totes, which are used directly to feed each batch reaction using specialty tote-to-process pumps. The process requires 1,619 gallons per week of benzyl alcohol, so 12 totes are purchased every two weeks. The process requires 805 gallons per week of acetic acid, so 6 totes are purchased every two weeks. It is assumed that the totes will be returned to the supplier; therefore, the cost of the totes is not included in the total storage costs.

ST-200 and ST-103 are considered intermediate tanks because they are constantly being filled and drained during the process. ST-200 is filled directly from the reactor outlet and is the source for continuous separations. ST-103 holds recycled unused reactants. A full inventory analysis was completed for ST-200 and ST-103 (see Process Description for details). ST-200 is 3,700 gallons and has a bare module cost of \$72,000. ST-103 is 2,600 gallons and has a bare module cost of \$50,000.

The storage tank volume for products was calculated on a two-week production basis. ST-201 holds wastewater before treatment; it has a volume of 550 gallons, which has a bare module cost of \$10,000. ST-203 holds dibenzyl ether before being sold; it has a volume of 300 gallons,

which has a bare module cost of \$5,000. ST-201 and ST-203 are transferred to 275-gallon totes for transportation. ST-201 uses 2 totes, and ST-203 uses 1 tote. The number of totes is doubled for costing purposes, so totes are always on site. This calculation assumes totes are returned by third parties. The cost of each tote is \$270.²⁰ ST-202 holds benzyl acetate before use as a feedstock to another process. ST-202 has a volume of 4,100 gallons, resulting in a bare module cost of \$78,000.

All storage tanks were costed using heuristics for floating-roof tanks and are made of stainless steel to prevent corrosion from acids, as shown in Appendix E-6.¹⁹ Additionally, the volume used for costing accounted for head space in the storage tank, which was assumed to be 10% of the liquid volume.

Table IV. Equipment List (Reactors, Pump, Distillation Columns)

Unit Number	Unit Type	Brief Function	Material of Construction	Size (Imperial)	Size (Metric)	Operating Conditions (T/P)
R-100	Slurry Batch Reactor	Endothermic reaction run in batches	Stainless Steel	D=1.47 ft H=34.6 ft V=58.6 ft ³	D=0.45 m H=10.5 m V=1.66 m ³	120°C 101.3 kPa
R-101	Horizontal Pressure Vessel	Regenerates catalyst by ramping up temperature	Stainless Steel	D=0.82 ft; L=1.75 ft; V=0.93 ft ³	D=0.25 m L=0.53 m V=0.026 m ³	350-500°C 101.3 kPa
P-100	External Gear Pump	Loads and unloads liquids from R-100	Stainless Steel	Q=777 gal/hr P=0.93 kW	Q=2939 L/hr P=0.93 kW	120°C 63.6 kPa
DT-200	Packed Bed Distillation Column	Separates water from other products/reactants	Stainless Steel	D=1.20 ft H _P =9.0 ft	D=0.37 m H _P =2.74 m	Condenser (100°C) Reboiler (200°C) 101.3 kPa
DT-201	Packed Bed Distillation Column	Separates unused reactants from products	Stainless Steel	D=2.41 ft H _P =70.5 ft	D=0.74 m H _P =21.5 m	Condenser (195°C) Reboiler (216°C) 101.3 kPa
DT-202	Packed Bed Distillation Column	Separates benzyl acetate from dibenzyl ether	Stainless Steel	D=0.53 ft H _P =7.5 ft	D=0.16 m H _P =2.29 m	Condenser (213°C) Reboiler (286°C) 101.3 kPa

Table V. Equipment List (Heat Exchangers)

Unit Number	Unit Type	Brief Function	Material of Construction	Size (Imperial)	Size (Metric)	Operating Conditions (T/P)
E-100	Double-Pipe Heat Exchanger	Pre-heats reactor feed	Stainless Steel	SA=11.6 ft ²	SA=1.08 m ²	25°C, 101.3 kPa
E-200	Double-Pipe Heat Exchanger	Cools reactor outlet for storage in ST-200	Stainless Steel	SA=51.5 ft ²	SA=1.86 m ²	25°C, 101.3 kPa
E-201	Double-Pipe Heat Exchanger	Cools wastewater for storage in ST-201	Stainless Steel	SA=2.83 ft ²	SA=0.10 m ²	25°C, 101.3 kPa
E-202	Double-Pipe Heat Exchanger	Cools recycled reactants for storage in ST-103	Stainless Steel	SA=34.7 ft ²	SA=1.25 m ²	25°C, 101.3 kPa
E-203	Double-Pipe Heat Exchanger	Cools benzyl acetate product for storage in ST-202	Stainless Steel	SA=13.2 ft ²	SA=0.48 m ²	25°C, 101.3 kPa
E-204	Double-Pipe Heat Exchanger	Cools dibenzyl ether product for storage in ST-203	Stainless Steel	SA=1.06 ft ²	SA=0.04 m ²	25°C, 101.3 kPa

Table VI. Equipment List (Storage Units)

Unit Number	Unit Type	Brief Function	Material of Construction	Size (Imperial)	Size (Metric)	Operating Conditions (T/P)
ST-101	Totes	Feeds fresh benzyl alcohol to system	HDPE	V=275 gal	V=1,040 L	25°C, 101.3 kPa
ST-102	Totes	Feeds fresh acetic acid to system	HDPE	V=275 gal	V=1,040 L	25°C, 101.3 kPa
ST-103	Intermediate Storage Tank	Holds recycled unused reactants	Stainless Steel	V=2,600 gal	V=9,842 L	25°C, 101.3 kPa
ST-200	Intermediate Storage Tank	Holds reactor batches to feed continuous separation	Stainless Steel	V=3,700 gal	V=14,006 L	25°C, 101.3 kPa
ST-201	Product Storage Tank/Totes	Holds wastewater to be sent to treatment	Stainless Steel HDPE	V=600 gal V=275 gal	V=2,019 L V=1,040 L	25°C, 101.3 kPa
ST-202	Product Storage Tank	Holds benzyl acetate product for another process	Stainless Steel	V=4,100 gal	V=15,198 L	25°C, 101.3 kPa
ST-203	Product Storage Tank/Totes	Holds dibenzyl ether product	Stainless Steel HDPE	V=300 gal V=275 gal	V=1,065 L V=1,040 L	25°C, 101.3 kPa

EQUIPMENT COST SUMMARY

Table VII. Equipment Cost Summary

	Unit Number	Unit Type	Purchase Price	Bare Module Cost	Source of Price	Notes
Reactor	R-100	Slurry Reactor	\$108,000	\$448,000	Design heuristics	Including factor for piping and circulation system & agitator
Pump	P-100	External Gear Pump	\$6,000	\$24,000	Design heuristics	Loading/unloading pump for reactor
Dist. Columns	D-200	Packed Bed Distillation Column	\$27,000	\$87,000	Design heuristics	Includes reboiler and condenser
	D-201	Packed Bed Distillation Column	\$168,000	\$675,000	Design heuristics	Includes reboiler and condenser
	D-202	Packed Bed Distillation Column	\$18,000	\$50,000	Design heuristics	Includes reboiler and condenser
HEX	E-100	Heat Exchanger	\$3,900	\$9,800	Design heuristics	-
	E-200	Heat Exchanger	\$6,400	\$11,000	Design heuristics	-
	E-201	Heat Exchanger	\$4,000	\$7,200	Design heuristics	-
	E-202	Heat Exchanger	\$6,000	\$10,800	Design heuristics	-
	E-203	Heat Exchanger	\$5,100	\$9,200	Design heuristics	-
	E-204	Heat Exchanger	\$3,400	\$6,200	Design heuristics	-
Storage	ST-101	Totes	\$0	\$0	Manufacturer quote ²⁰	Returned to the provider
	ST-102	Totes	\$0	\$0	Manufacturer quote ²⁰	Returned to the provider
	ST-103	Intermediate Storage Tank	\$16,000	\$50,000	Design heuristics	-
	ST-200	Intermediate Storage Tank	\$23,000	\$72,000	Design heuristics	-
	ST-201	Product Storage Tank	\$3,400	\$10,000	Design heuristics	Combination of storage vessel and totes
	ST-201	Totes	\$1,100	\$1,600	Manufacturer quote ²⁰	Combination of storage vessel and totes
	ST-202	Product Storage Tank	\$26,000	\$78,000	Design heuristics	-
	ST-203	Product Storage Tank	\$1,800	\$5,500	Design heuristics	Combination of storage vessel and totes
	ST-203	Totes	\$500	\$800	Manufacturer quote ²⁰	Combination of storage vessel and totes

FIXED-CAPITAL INVESTMENT SUMMARY

Table VIII. Total Capital Investment

Cost	Amount	Assumptions
C_{TCI}	\$3,500,000	
C _{WC}	\$300,000	10% of C _{TPI}
C _{TPI}	\$3,200,000	
C _{startup}	\$300,000	10% C _{TDC}
C _{royal}	\$0	Assume none, no patents used
C _{land}	\$0	Assume negligible
C _{TDC}	\$2,900,000	
C _{contingency}	\$264,000	10% C _{DPI}
C _{DPI}	\$2,650,000	
C _{alloc}	\$928,000	Installation of hot oil, chilled water, and electrical systems
C _{serv}	\$40,000	50% C _{site}
C _{site}	\$80,000	Integrated plant (5% C _{TBM})
C _{TBM}	\$1,600,000	
C _{PM}	\$1,350,000	Includes reactor, distillation columns, hex, loading pump, and regen.
C _{spare}	\$24,000	Includes one spare pump for reactor unloading/loading
C _{initial}	\$5,000	Includes catalyst for 1 st year & feedstock for first 3 batches of the yr.
C _{storage}	\$218,000	Includes intermediate tanks, product storage tanks & totes

SAFETY AND ENVIRONMENTAL

Background

In recent years environmental protection and safety has changed from a secondary to a primary issue in industries.²¹ Major capital and managerial investments have been made within the chemical industry to minimize sources of pollution and mitigate common safety risks.²¹ In order to maintain a good company reputation and reduce the risk of any chemical accidents, both the safety and environmental aspects of a plant should be closely monitored.

Safety Overview

The feedstocks of the process are benzyl alcohol and acetic acid, and the products are benzyl acetate, dibenzyl ether, and water. Benzyl alcohol, dibenzyl ether, and benzyl acetate are all mild skin and eye irritants.^{7,8,9} Acetic acid is a Category 1 corrosive that can cause serious eye and skin damage according to the Globally Harmonized System (GHS) scale.⁶ Therefore, materials such as stainless steel are used to ensure piping does not experience corrosion and/or leaks that could ultimately result in acetic acid exposure to employees within the facility. The exposure of acetic acid to pipes is also limited by the design of our reactor, which uses benzyl alcohol as the excess reactant and acetic acid as the limiting reactant with high conversion. The zeolite being used (HZSM-5) is a skin and eye irritant, so appropriate personal protection equipment (PPE) such as gloves and eye protection should be worn when handling.²² Note that this safety precaution is advisable during the transfer process of catalyst between the reactor and regeneration unit.²² Overall, there are no known carcinogenic effects of these chemicals.^{6,7,8,9}

As shown in Table IX, most compounds have a low TLV-TWA of 10 ppm, which could pose safety hazards to operators if these chemicals are vaporized and released within the facility. To minimize this risk, all streams in the plant should be maintained at 25°C or lower to prevent partial vaporization of these toxic chemicals. This safety risk is one of the major reasons the five coolers (E-200, E-201, E-202, E-203, and E-204) are part of the final design. Fortunately, all components used in the process have very low vapor pressures (less than 25 mmHg) at 25°C.^{6,7,8,9} Furthermore, due to the facility being indoors, proper ventilation and extraction systems must be in place in the case of an unexpected release of toxic vapor. One add-on piece of equipment that could be implemented is a thermal incinerator, which burns organic vapors of the volatile components before pressure can be built up within a vessel. These systems typically have a burn efficiency of at least 98%.²³

Another consideration is the high temperatures associated with the reactor (up to 120°C), the hot oil recirculation system (up to 340°C), and the regeneration unit (up to 550°C). Proper PPE such as temperature resistance gloves and boots should be used when working close to this equipment. Additionally, when conducting maintenance inspections, proper lockout/tagout procedures need to be in place to ensure that operators will not get burned by touching any hot pipes or metal encasings. These procedures should also be applied to any other units requiring maintenance within the plant.

Other important safety issues are fires and explosion hazards. Several chemical plant accidents can be attributed to the accumulation of flammable chemicals in air resulting in ignition.²¹ Flammability metrics, such as the lower flammability limit (LFL) and the upper flammability limit (UFL), are utilized to determine potential fire and explosion hazards in a chemical process. As seen in Table IX, all the chemicals have very high auto ignition temperatures but only moderate flash points and flammability ranges. The high auto ignition temperatures will help prevent any explosion from happening in the reactor, which is operating at 120°C. However, the flash points and flammability ranges are within ranges that suggest they should be closely monitored. Additionally, it should be noted that the hot oil is operating above its fire point, which is the temperature at which a flame can be sustained with an outside source of ignition. Therefore, it must be ensured that the fluid is never in contact with air and that all pipes are well insulated to minimize potential nearby ignition sources. In order to prevent a potential fire from occurring, components are stored under atmospheric conditions of 25°C and 1 atm to reduce any build-up of vapor that could potentially ignite. To further lower the probability of ignition, procedures such as nitrogen inerting or induction charging could be implemented.²¹ Also, general housekeeping procedures should be followed to ensure electrical equipment and wiring is not in a location that could be disastrous for the plant.

Finally, storage is a major part of the plant due to its unique design, combining a reactor batch process with a continuous separation. Therefore, intermediate storage tanks should be closely monitored to ensure they do not become empty or overflow. Specifically, ST-200 should maintain a minimum liquid volume of 3,000 L to prevent the continuous distillation columns from running dry. On the other end, ST-103 should not exceed a liquid volume of 9,300 L to prevent the tank from overflowing as it is a direct output of continuous distillation. While these tanks are the most critical, high-level and low-level alarms should be installed on all tanks to warn operators of any volume limits that are being approached. All storage tanks should also have carefully designed overflow pipes in case the level alarms are not working properly.

Table IX. Safety Parameters of Chemicals^{6,7,8,9,24}

Chemical	LFL (% vol)	UFL (% vol)	Flash Point (°C)	Fire Point (°C)	Auto Ignition (°C)	TLV-TWA (ppm)
Acetic Acid	4	19.9	39-43	-	463	10
Benzyl Alcohol	1.3	13	96	-	435	10
Benzyl Acetate	0.9	8.4	90	-	460	10
Dibenzyl Ether	-	-	135	-	470	-
Heating Oil	1.4	7.8	220	255	450	-

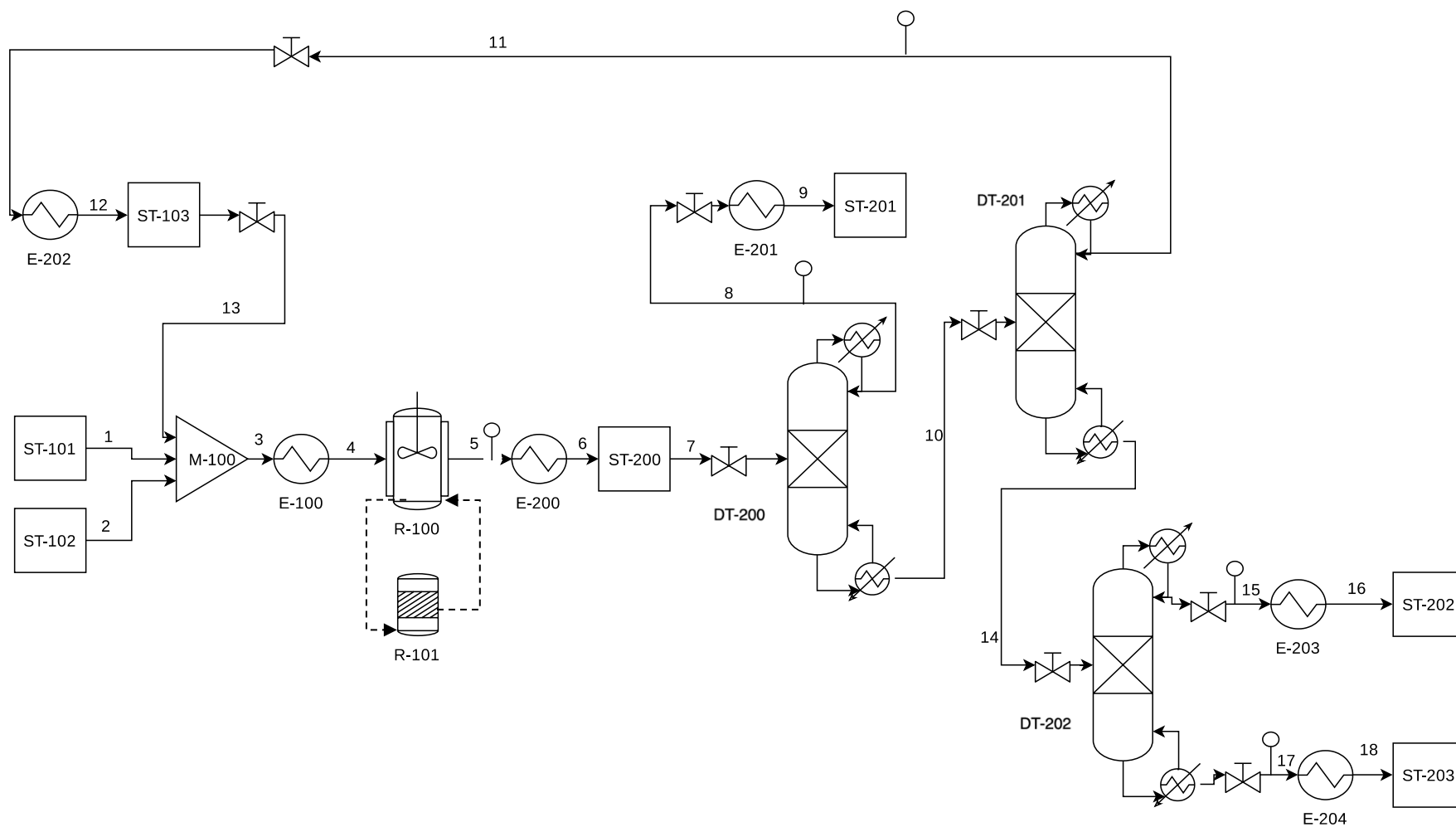


Figure 10. P&ID of Process to Produce Benzyl Acetate

Process Control & Risk Analysis

As shown on the P&ID in Figure 10, composition analyzers are installed on certain streams within the process in order to help achieve desired stream purities. The five critical streams are: (1) the outlet of R-100, (2) the distillate of DT-200, (3) the distillate of DT-201, (4) the distillate of DT-202 and (5) the bottoms of DT-202. Monitoring the distillate of DT-200 is crucial to ensure a mass purity of 96% for water is achieved. It is important to maintain the mass purity of approximately 99% of benzyl alcohol in the distillate of DT-201 so that the recycle can be assumed as pure. Lastly, the distillate and bottoms streams from DT-202, benzyl acetate and dibenzyl ether product streams, must maintain their 99% purities in order to be used as a feedstock and sold, respectively. While the benzyl acetate stream is permitted to be as low as 96% with 4% benzyl alcohol, meeting this specification would lead to a decrease the purity of our recycle streams. One way to maintain the benzyl acetate product purity within $\pm 0.5\%$ is to set up a feedback loop between the DT-202 distillate analyzer and the DT-202 reflux valve. If the analyzer senses a low purity, a signal will be sent to increase the reflux ratio. Because a higher reflux ratio will result in more vapor-liquid mass transfer, this arrangement is one way to ensure the distillate stream will return to its typical purity.

A general risk summary was conducted on the proposed process design to identify possible hazards and rank their significance using safety heuristics such as operating temperatures, operating pressures, and inherent safety of the chemicals involved within each unit. For each section of the P&ID, expected hazards were noted, considering both their expected degree of severity expected degree of likelihood.

The section with the highest risk is expected to be the reactor (streams 5 and 6) due a combination of several factors: large batch size, high operating temperature, handling of corrosive acetic acid, and complexity. As part of its complexity, it has a heating jacket that requires a large flowrate of hot oil to be flowing through the jacket during the reaction and an agitator that requires a supply of electricity. Therefore, a detailed hazard and operability (HAZOP) study was conducted on the reactor, as shown as Table X.²⁵

The first potential issue examined is the possibility for the heating jacket of the reactor to supply more energy to the reactor than expected due to a failure in the supply control valve. This issue can lead to an increase of temperature and pressure, which has the potential to cause an explosion. Ventilation systems (including rupture disks and relief valves) or a thermal incinerator could be installed to prevent this build-up of pressure. Additionally, temperature and pressure alarms should be installed on the reactor to make operators aware of this potential issue. The second issue considered concerns the agitator. Lack of mixing will lead to a lower conversion of acetic acid as the kinetic parameters depend on the agitator running at 200 rpm. A different problem will occur if too much power is supplied to the agitator, which could lead to an electrical fault, shutting it down. The last issue considered is the liquid fraction of acetic acid in the reactor. While it is unlikely for the acetic acid to corrode the stainless-steel vessel, this could potentially lead to the formation of leaks over time, which could present a danger to any operators in the area if exposed to the acid. Possible consequences and recommended actions associated with these issues are summarized in Table X below.

Table X. HAZOP Study on the Reactor (R-100) ²⁵

Unit	Process Parameter	Guide Word	Possible Causes	Possible Consequences	Recommended Actions
Heating Jacket in Batch Reactor	Flow	NONE	1. Control valve fails to open 2. Hot oil system fails (pipe blockage or rupture)	1. Decrease in temperature of the reaction; less acetic acid conversion	1. Regular maintenance 2. Check hot oil system reliability 3. Install flow and temperature analyzers on hot oil stream 4. Install ventilation systems (rupture disks, relief valves) or a thermal incinerator
		MORE OF	1. Control valve fails to close	1. Unsafe operating temperature and pressure; lower BAc selectivity 2. Explosion caused by pressure build-up	
		LESS OF	1. Control valve fails to respond 2. Hot oil leakage	1. Decrease in temperature of the reaction; less acetic acid conversion	
	Temperature	MORE OF	1. High hot oil supply temperature	1. Unsafe operating temperature and pressure; lower BAc selectivity 2. Explosion caused by pressure build-up	1. Install ventilation systems (rupture disks, relief valves) or a thermal incinerator 2. Install high and low temperature alarm
		LESS OF	1. Low hot oil supply temperature	1. Decrease in temperature of the reaction; less acetic acid conversion	
Agitator in the Batch Reactor	Mixing	NONE	1. Stirrer motor malfunction 2. Power failure	1. No mixing; lower acetic acid conversion	1. Install analyzers that monitor stirring rate and associated alarms for high stirring rates 2. Manual shutdown if agitator exceeds a certain rotational speed threshold
		MORE OF	1. Stirrer motor controller fails, resulting in high motor speed	1. Electrical fault and shut down	
R-100 Reactor Vessel	Mass Fraction of Acetic Acid	MORE OF	1. Allowing acetic acid to sit in reactor alone 2. Lower conversion	1. Corrosion of vessel 2. Leaks to process facility	1. Add benzyl alcohol before acetic acid 2. Use stainless steel

In conclusion, most of the safety concerns are related to the toxicity and flammability of compounds used throughout the process. Therefore, the safety focus should be on having regular equipment inspections and ensuring proper PPE usage.

Environmental Overview

Environmental protection is a major factor when designing a new plant or integrating a new process into an already existing plant. All the compounds within the process, except water, have a high level of aquatic toxicity and should not be released into the environment. Benzyl alcohol and dibenzyl ether have a particularly severe aquatic toxicity, with values of 55 mg/L and 2.2 mg/L, respectively.^{7,9} Therefore, it is critical to ensure that these chemicals do not leak into any sewer drains within the facility. Because a recycle stream was implemented in the design, all the unused reactants are sent back to the feed streams, minimizing the liquid waste disposal of the plant. However, leakage is still possible from pipes, likely a result of corrosion from acetic acid. As previously mentioned, however, the reactor conditions chosen allow acetic acid to be the limiting reactant with a high conversion. Therefore, the amount of acetic acid in the recycle stream and remainder of the process is limited. Even with these precautions, sewer guards should be implemented to ensure any leaked chemicals do not enter natural waterways.

Water, a byproduct of the reaction, requires investment in wastewater treatment since the purity of water being discarded, about 96% by mass, cannot be released into the environment. The wastewater impurities consist of benzyl alcohol and acetic acid. While benzyl alcohol is not explicitly listed as a controlled substance under the Clean Water Act (CWA), acetic acid is directly regulated under CWA 311-HS, which requires reporting of any substance released into navigable waterways.¹⁰ Therefore, the water should be sent to a wastewater treatment facility to ensure that no waste is being disposed of incorrectly and that all bodies of water around the plant will fit the water quality criteria of the EPA. The disposal of the catalyst must also be closely considered and should be treated before disposal in a proper container under the Resource Conservation and Recovery Act (RCRA).²⁶

All the chemicals used in this process are listed as part of the Toxic Substance Control Act (TOSCA) Inventory. TOSCA reporting regulations apply directly to imported chemicals and any products being produced at more than 25,000 pounds per year.¹¹ Therefore, acetic acid and benzyl alcohol must be closely tracked if they are imported from outside the U.S. Additionally, dibenzyl ether and benzyl acetate are produced in large enough quantities that they should be closely monitored. The EPA requires specific reporting for each of these chemicals and regular inspections of facilities every four years.¹⁰ Therefore, it is important to keep detailed records of inventory throughout every operating year. On the other hand, none of these chemicals are considered hazardous air pollutants (HAPs) by the EPA.¹² In fact, one of the main environmental advantages of this process is that the reaction does not directly produce any methane or carbon dioxide. The only source of indirect air pollution is the burning of natural gas, which is required to heat the hot oil recirculation system and provide electricity. Another major benefit is that this process has a low solvent intensity because diluents and solvents are not required, as would be the case if liquid-liquid extraction was used for separation. For a fair assessment of the environmental impact of this process, a full life cycle analysis (LCA) should be performed.

OPERATING COST AND ECONOMIC ANALYSIS

Operating Cost

The economic analysis refers to Tables XI-XIV, presented below. Table XI provides an overview of all expected operating costs required for the plant.

Table XI. Operating Costs Summary

Cost	Amount	Assumptions
C _{operating}	\$1,700,000	Sum of COM and GE
Cost of Manufacture (COM)	\$1,700,000	
Feedstocks	\$773,000	
Catalysts	\$300	Replacement assumed to be every 10 wks
Utilities	\$103,000	See Table XIII
Operations	\$290,000	
DW&B	\$240,000	Assume \$40/hr, 1 operator/shift, 750 shifts/yr
DS&B	\$36,000	15% of DW&B
Operating Supplies and Services	\$14,000	6% of DW&B
Tech. Assist. to Manufacturing	\$0	Assume negligible
Control Laboratory	\$0	Assume no control lab
Maintenance	\$234,000	
MW&B	\$102,000	3.5% of C _{TDC} , fluid handling process
Salaries and Benefits	\$25,000	25% of MW&B
Materials and Services	\$102,000	100% of MW&B
Maintenance Overhead	\$5,000	5% of MW&B
Operating Overhead	\$94,000	
General Plant Overhead	\$29,000	7.1% of M&O-SW&B
Mechanical Dept. Services	\$10,000	2.4% of M&O-SW&B
Employee Relations Dept.	\$25,000	5.9% of M&O-SW&B
Business Services	\$30,000	7.4% of M&O-SW&B
Property Taxes & Insurance	\$0	Assume already considered for plant
Depreciation	\$211,000	
Direct Plant	\$145,000	8% of (C _{TDC} - 1.18C _{alloc})
Allocated Plant	\$66,000	6% of 1.18C _{alloc}
Rental Fees	\$0	Assume already considered for plant
Licensing Fees	\$0	Assume negligible
General Expense (GE)	\$1,600	
Selling Expense	\$400	3% of DBE sales
Direct Research	\$600	4.8% of DBE sales
Allocated Research	\$100	0.5% of DBE sales
Administrative Expense	\$300	2.0% of DBE sales
Mgt. Incentive Compensation	\$200	1.25% of DBE sales

Table XII below provides a summary of all the costs required for each chemical.

Table XII. Key Chemical Costs

Chemical	Amount (\$/kg)
Acetic Acid	\$0.66
Benzyl Alcohol	\$2.10
Zeolite Catalyst	\$3.00
Dibenzyl Ether	\$0.48

Table XIII breaks down the individual utility costs for each unit within the plant.

Table XIII. Utility Cost Summary

Unit	Required Utility	Cost (\$/yr)
Total	Multiple	\$103,000
R-100	Multiple	\$1,400
Heating Jacket	Hot Silicon Oil	\$1,000
Catalyst	Solid Waste Treatment	\$190
Agitator	Electricity	\$30
Pump	Electricity	\$180
R-101	Electricity	\$600
D-200	Multiple	\$8,800
Condenser	Chilled Water	\$2,000
Reboiler	Hot Silicon Oil	\$6,800
D-201	Multiple	\$74,600
Condenser	Chilled Water	\$39,300
Reboiler	Hot Silicon Oil	\$35,300
D-202	Multiple	\$3,600
Condenser	Chilled Water	\$1,900
Reboiler	Hot Silicon Oil	\$1,700
E-100	Hot Silicon Oil	\$1,200
E-200	Chilled Water	\$1,700
E-201	Chilled Water	\$140
E-202	Chilled Water	\$2,900
E-203	Chilled Water	\$1,200
E-204	Chilled Water	\$120
ST-201	Wastewater Treatment	\$6,900

Lastly, Table XIV below provides a summary of all the unit costs required for each utility.

Table XIV. Key Utility Costs

Utility	Cost	Units
Electricity	\$0.07	kWh
Natural Gas (to Heat Hot Silicon Oil)	\$4	MMBtu
Wastewater Treatment	\$0.45	gallon
Solid Waste	\$150	ton
Chilled Water	\$1.50	ton-day

Background

Even though benzyl acetate is not being sold due to its use in a downstream process, it is valuable to know the theoretical sales price of benzyl acetate necessary to achieve a certain internal rate of return (IRR), assumed to be 15% for this analysis. Currently, benzyl acetate is being bought from a supplier at a price of \$6.40/kg. Therefore, if the theoretical benzyl acetate price is determined to be well under \$6.40/kg, it is recommended to proceed with the construction of a plant. However, if the theoretical price is determined to be similar to or greater than \$6.40/kg, it is recommended to continue purchasing benzyl acetate from the current supplier. For this analysis, the plant is assumed to be an integrated plant with a lifetime of twenty years.

Economic Analysis

First, the theoretical annual sales (S) must be determined by summing the total annual theoretical sales of benzyl acetate with the total annual expected sales of dibenzyl ether. Because the BAc price (P_{BAC}) must be adjusted after the completion of the full economic analysis, it was left as a variable. However, the price of DBE (P_{DBE}) was assumed to be \$0.48/kg, a conservative estimate determined by dividing the cost of a single kilogram on Sigma-Aldrich by a factor of 100.²⁷ The theoretical annual sales of benzyl acetate and dibenzyl ether was then summed using the formula below:

$$S = P_{BAC}\dot{m}_{BAC} + P_{DBE}\dot{m}_{DBE}$$

$$S = P_{BAC}(400,000 \text{ kg/yr}) + (\$0.48/\text{kg})(28,000 \text{ kg/yr})$$

Depreciation values were then determined using a Modified Accelerated Cost Recovery System (MACRS) for the first 10 operating years of the plant using the following formula:

$$D_n = (C_{TDC} - S_v) \times \frac{d_n}{100}$$

where C_{TDC} is the total depreciable capital, S_v is the salvage value expected at the project's end, n is the operating year being considered (i.e. year 1 is 2021), and d_n is the depreciation associated

with the 10-year MACRS schedule. The value of C_{TDC} is \$2.9 million, as outlined in Table XIII. The value of S_v is assumed to be 5% of C_{TDC} , or \$145,000.

Once the depreciation is determined for each year, the cash flow (CF) values are determined for each year using the formula below:

$$CF_n = (1 - t)(S - C) + D_n - C_{TCL,n} + S_{v,n}$$

where t is the tax rate of 27% (21% federal and 6% Georgia), C is the operating cost determined to be \$1.7 million in Table XI, and all other variables have been previously defined. Note that $C_{TCL,n}$ is zero for every year except 2020, where it is \$3.5 million, as shown in Table XV. Similarly, $S_{v,n}$ is zero for every year but 2041, where it is \$145,000.

The cash flow values must then be discounted to account for inflation (f) and to account for a discount rate (i), which essentially is the interest rate an investor is assumed to receive upon keeping the capital in other financial assets, such as stocks, bonds, or bank accounts. Because building a chemical plant is a major investment, a higher than expected value is typically given to the discount rate to account for the risk. The formula for DCF is defined as:

$$DCF_n = (CF_n - D_n) \left(\frac{1 + f}{1 + i} \right)^n + D_n \left(\frac{1}{1 + i} \right)^n$$

where the inflation rate (f) is assumed to be 3% and the discount rate (i) is assumed to be 15%. The discounted cash flows for each year can then be summed to determine the net present value, as shown below:

$$NPV = \sum_{n=0}^{21} DCF_n$$

Under the assumption that BAc is sold at \$6.40/kg, a positive NPV of \$2.9 million is achieved, which suggests that the building of the plant is likely to be profitable, as shown in Figure 11.

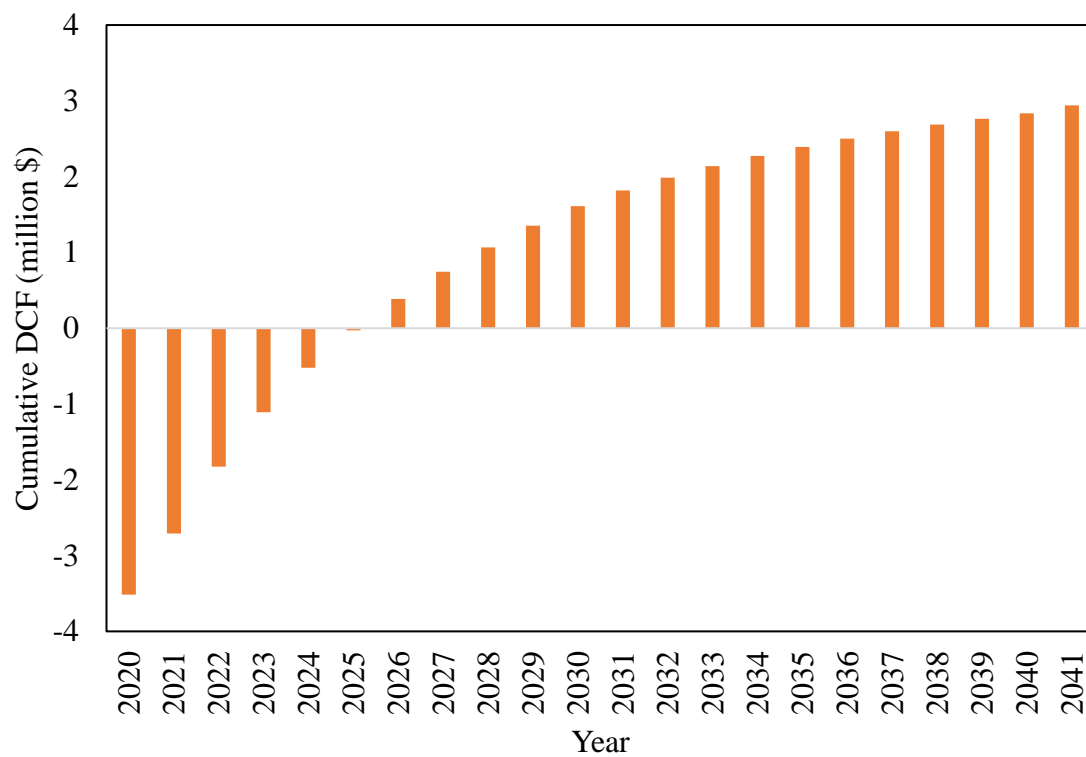


Figure 11. Theoretical Cumulative Discounted Cash Flow If Benzyl Acetate Was Being Sold at \$6.40/kg

Similarly, a cash flow spreadsheet was developed under the theoretical assumption that benzyl acetate is sold for \$6.40/kg, as shown in Table XV.

Table XV. Theoretical Discounted Cash Flow Sheet If Benzyl Acetate Was Being Sold at \$6.40/kg

NOTE: All values are presented in millions

Actual Year	Year	Capital Cost	Operating Cost	Sales	MACRS%	Depreciation	Salvage	Cash Flow	DCF
2020	0	\$3.52	\$0.00	\$0.00	0%	\$0.00	\$ -	-\$3.52	-\$3.52
2021	1	\$ -	\$1.70	\$2.56	10%	\$0.28	\$ -	\$0.90	\$0.80
2022	2	\$ -	\$1.70	\$2.56	18%	\$0.50	\$ -	\$1.12	\$0.88
2023	3	\$ -	\$1.70	\$2.56	14.40%	\$0.40	\$ -	\$1.02	\$0.71
2024	4	\$ -	\$1.70	\$2.56	11.52%	\$0.32	\$ -	\$0.94	\$0.58
2025	5	\$ -	\$1.70	\$2.56	9.22%	\$0.25	\$ -	\$0.88	\$0.49
2026	6	\$ -	\$1.70	\$2.56	7.37%	\$0.20	\$ -	\$0.83	\$0.41
2027	7	\$ -	\$1.70	\$2.56	6.55%	\$0.18	\$ -	\$0.81	\$0.36
2028	8	\$ -	\$1.70	\$2.56	6.55%	\$0.18	\$ -	\$0.81	\$0.32
2029	9	\$ -	\$1.70	\$2.56	6.56%	\$0.18	\$ -	\$0.81	\$0.28
2030	10	\$ -	\$1.70	\$2.56	6.55%	\$0.18	\$ -	\$0.81	\$0.25
2031	11	\$ -	\$1.70	\$2.56	3.28%	\$0.09	\$ -	\$0.71	\$0.21
2032	12	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.17
2033	13	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.15
2034	14	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.13
2035	15	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.12
2036	16	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.11
2037	17	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.10
2038	18	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.09
2039	19	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.08
2040	20	\$ -	\$1.70	\$2.56	0%	\$ -	\$ -	\$0.62	\$0.07
2041	21	-\$0.32	\$1.70	\$2.56	0%	\$ -	\$0.15	\$1.09	\$0.11
								NPV	\$2.88

Decision

While it is valuable to see the NPV that would be achieved at a benzyl acetate sale price of \$6.40/kg, it is also valuable to determine the theoretical sale price of benzyl acetate needed to give an IRR of 15%, found by adjusting P_{BAC} until an NPV of zero is achieved. After completing the full economic analysis shown above, an IRR of 15% can be achieved at a benzyl acetate sale price of \$5.10/kg, which is 20% lower than the \$6.40/kg required to buy it from the current supplier. Therefore, we recommend proceeding with the construction of the benzyl acetate production plant. Over the course of twenty years, this difference results in a savings of approximately \$10.4 million as calculated below:

$$Savings = \dot{m}_{BAC} t_{lifetime} (P_{BAC, supplier} - P_{BAC})$$

$$Savings = (400,000 \text{ kg BAC/yr})(20 \text{ yrs})(\$6.40 - \$5.10)$$

$$Savings = \$10.4 \text{ million}$$

Sensitivity Analysis

Due to the extensive amount of the assumptions involved in the economic analysis, it is valuable to assess the sensitivity of certain design decisions on the theoretical benzyl acetate price. The five major decisions that will be analyzed include: the selling price of dibenzyl ether, the inclusion of heat integration, the inclusion of a control laboratory, the rate of catalyst replacement, and the number of operators hired per shift. Additionally, to account for any approximations used in the design of individual units, the effect of altering major capital costs on the theoretical price of benzyl acetate is reported.

The baseline assumption for our design is that dibenzyl ether is sold at \$0.48/kg, which results in our theoretical BAc price of \$5.10/kg. However, it is important to note that the amount of dibenzyl ether produced (28,000 kg/year) is minimal in comparison to BAc (400,000 kg/year). While selling the dibenzyl ether is still a more profitable approach, failure to sell the dibenzyl ether will result in a theoretical BAc price of \$5.12/kg, an increase of only \$0.02/kg. Therefore, the sale of dibenzyl ether is not critical to the profitability of our design. However, if a higher market price does become known, the sale of dibenzyl ether would likely become more worthwhile, as depicted by the decreasing trend in Figure 12.

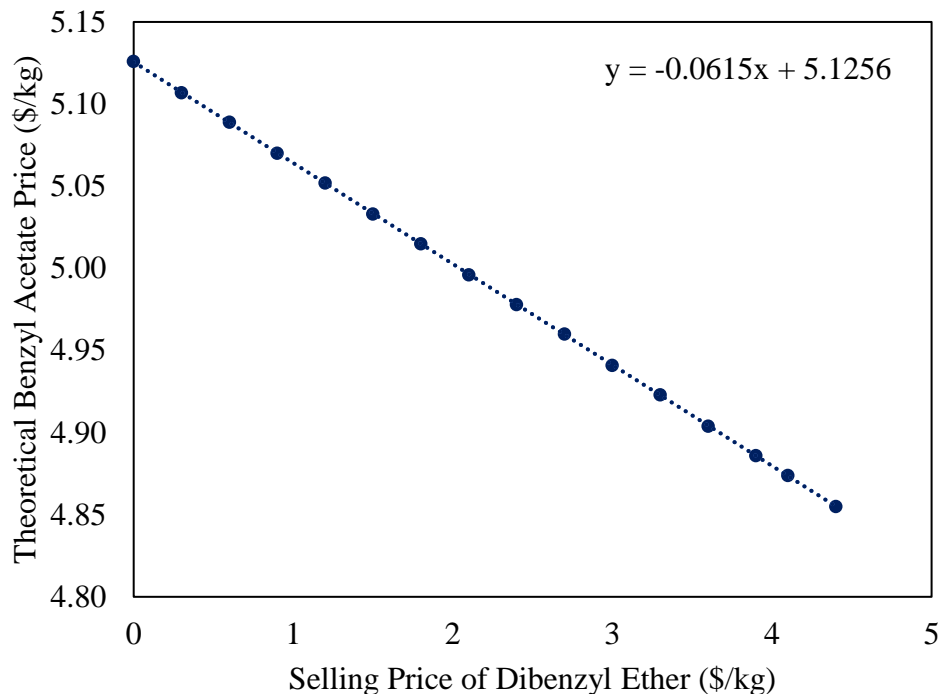


Figure 12. Sensitivity of Dibenzyl Ether Selling Price

Next, the decision not to move forward with heat integration is outlined in the energy balance and utility requirements section of the report. While utilities costs drop by \$3,700/yr, the capital cost of the heat exchangers increase by \$13,000. The overall result is that the theoretical benzyl acetate price remains unchanged at \$5.10/kg.

For the control lab, the baseline assumption is that a control lab is not necessary due to the use of composition analyzers on the critical streams within the process. However, if a control lab was required, design heuristics suggest it would cost \$65,000/(operators/shift)/yr, or \$65,000/year given that only one operator is assumed per shift. This addition would change the theoretical BAC price from \$5.10/kg to \$5.26/kg, a moderate increase in the price. Therefore, it is not suggested to implement a control laboratory—at least one of that scale.

Because our catalyst is in a slurry batch reactor, the rotating turbine is likely to wear down the catalyst at a faster rate than would be seen in a packed bed reactor (PBR), resulting in a higher catalyst replacement rate. The deterioration of the catalyst requires buying new catalyst and disposing of spent catalyst, both of which are considered in this analysis. As can be seen in Figure 13, the theoretical price of benzyl acetate is marginally affected by changes in catalyst replacement rate, likely a result of the low amounts of catalyst needed per batch and the low cost of the catalyst. For instance, catalyst replacement every week results in a theoretical BAC value of \$5.12/kg, while catalyst replacement every 4 years results in a theoretical BAC value of \$5.10/kg. Our baseline assumption was chosen to be a catalyst replacement rate every 10 weeks because it results in the low theoretical BAC value of \$5.10/kg while mitigating any risk associated with loss of catalyst activity over time.

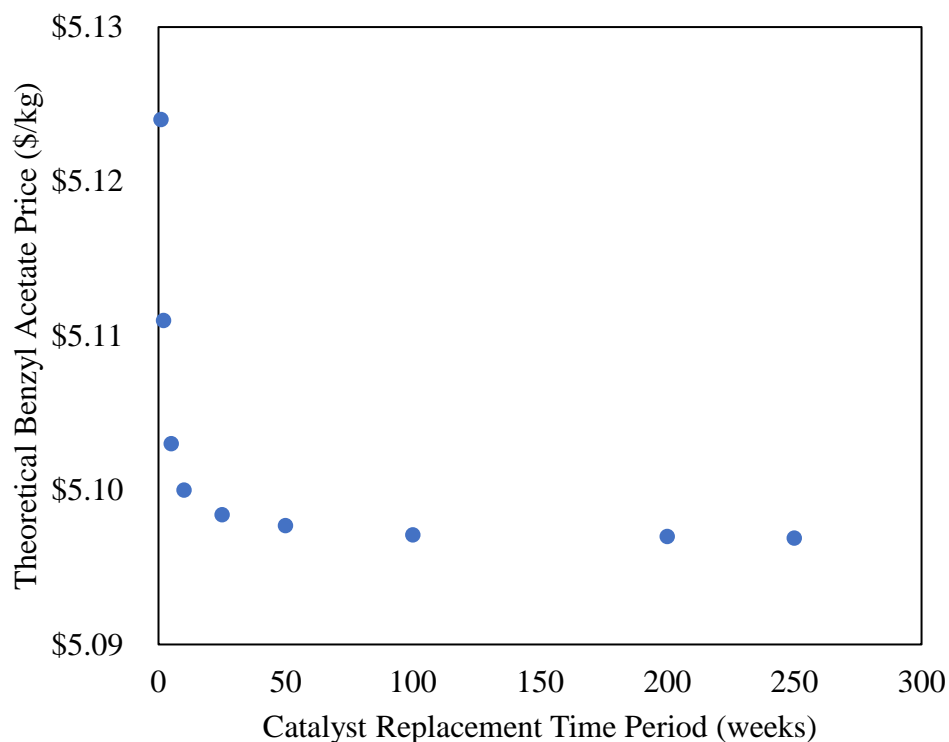


Figure 13. *Sensitivity of Catalyst Replacement Rate*

Finally, it is crucial to consider the effect of hiring additional operators because additional labor is expensive. In this analysis, the baseline assumption is that there is only one operator per eight-hour shift required in addition to the current staff. Each operator receives direct wages and benefits equivalent to \$40/hr. Based on Figure 14 below, each additional operator increases the theoretical BAc price by \$0.88/kg. Therefore, it is possible to hire either one or two operators per shift and maintain profitability of the plant. However, we recommend proceeding with only one additional operator per shift in addition to the current staff in order to achieve the higher profitability.

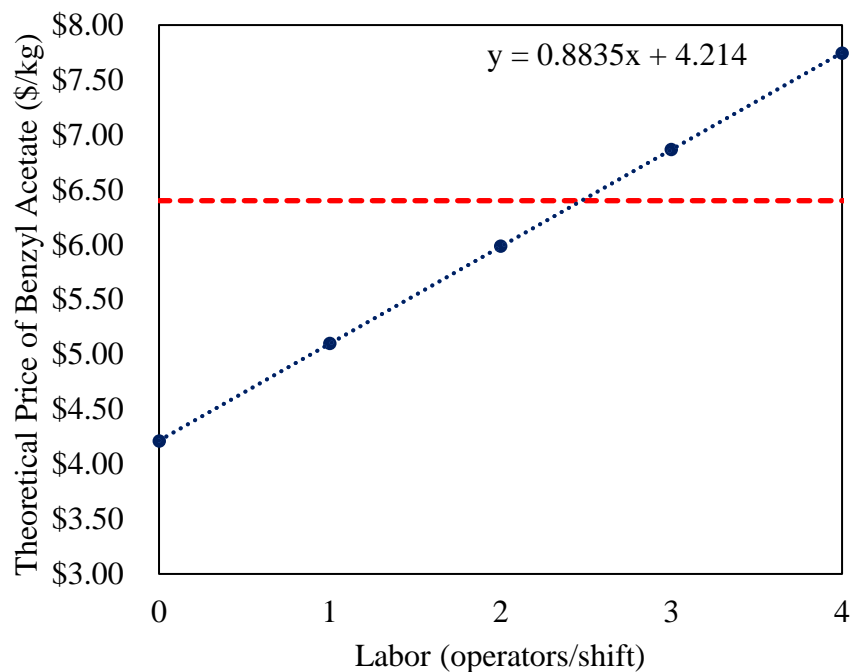


Figure 14. Sensitivity of Number of Operators

In addition to the factors presented above, the sensitivities of major unit equipment costs are analyzed. Figure 15 analyzes how the cost of the major units in the plant affect the overall profitability. Changes in the cost of distillation columns is most sensitive because it accounts for 62% of the plant's capital cost.

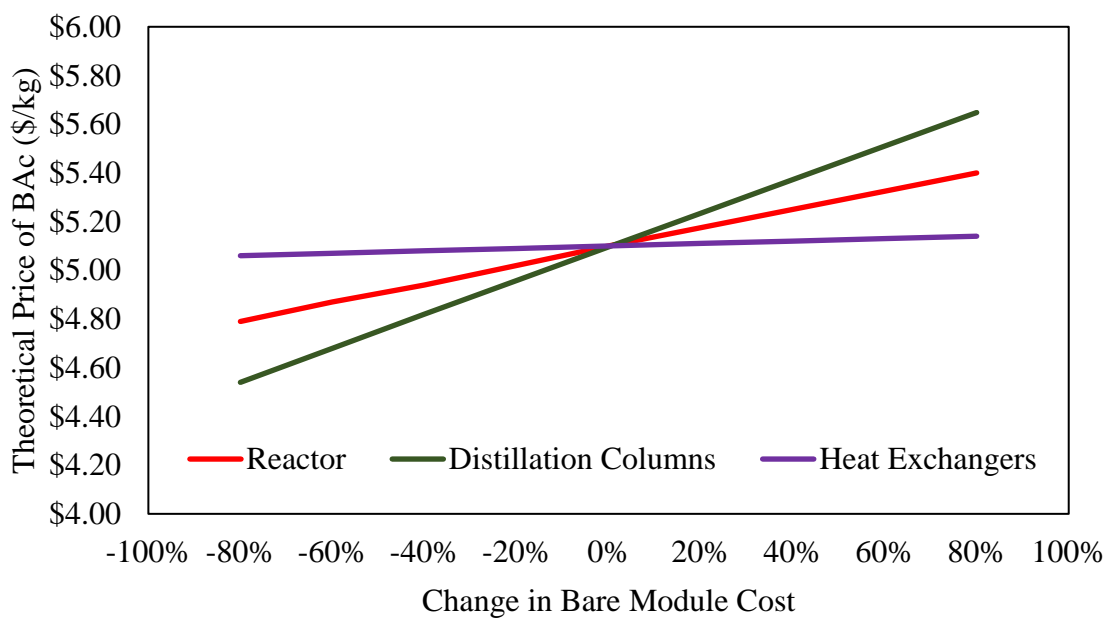


Figure 15. Sensitivity of Major Unit Costs

One final note is that the baseline assumption assumes a discount rate of 15%, meaning that the profitability of the plant must have an IRR of 15% in order to be considered for construction. However, if the discount rate is assumed to be 10%, the theoretical benzyl acetate price could be as low as \$4.73/kg. Conversely, if the discount rate is assumed to be 20%, the theoretical benzyl acetate price could be as high as \$5.52/kg. While neither of these assumptions affect the decision to construct the benzyl acetate plant, the effect is substantial enough that it should not be neglected.

Overall, we determined that the rate of catalyst replacement and the incorporation of heat integration both had nominal effects on the profitability of the plant. In contrast, the selling price of DBE and the addition of the control lab could affect the theoretical benzyl acetate price by \$0.35/kg. Most importantly, the number of hired operators and the cost of the distillation columns were the two major variables that are likely to be sensitive enough in the analysis to potentially affect the final decision. Fortunately, the number of operators can be easily controlled as a management decision. However, the exact cost of the distillation columns, particularly DT-201, may not be known ahead of time. Therefore, we recommend getting a quote for a packed distillation column with the dimensions and material of DT-201 to ensure it falls below \$1.2 million. This value is determined by assuming the construction of the plant is break-even if the worst-case scenario for all examined factors is realized. While the worst-case scenario is unlikely, the recommendation to continue with the implementation of the plant assumes that the estimated cost of DT-201 is validated.

CONCLUSIONS AND RECOMMENDATIONS

Overall, we recommend proceeding with the implementation of the benzyl acetate production plant. The desired annual production rate of 100,000 gallons of benzyl acetate with a mass purity of 99% is achieved in the process design. Specifically, the annual production of benzyl acetate is 100,500 gallons at 99.4% purity, which is stored until its use in a downstream process. Additionally, the byproduct of the reaction, dibenzyl ether, was produced at an annual rate of 7,000 gallons with 99% purity by mass and is ultimately sold.

The total capital investment required for this project is \$3.5 million and the annual operating required is \$1.7 million. Based on a full economic analysis, the theoretical sales price of benzyl acetate necessary to achieve an IRR of 15% is \$5.10/kg, which is 20% lower than the \$6.40/kg required from the current provider. Ultimately, this project results in a lifetime savings of \$10.4 million over the course of the twenty years.

For this design, the major loss of energy occurs at the separation of benzyl acetate from unused benzyl alcohol in DT-201. This distillation column consumes approximately 75% of both heating and cooling requirements within the plant. If acetic acid is fed in excess instead of benzyl alcohol, the intensity of this separation would drop as benzyl alcohol will be mainly consumed in the reaction. However, this will result in a harder separation between water and acetic acid in DT-200. Additionally, this decision would cause acetic acid to be present throughout the plant, including in the recycle stream and ST-103, increasing the likelihood of a potential worker exposure. Lastly, heat integration is not recommended due to the added process complexity as it has no effect on the theoretical price of benzyl acetate nor the lifetime savings of the project.

Because our analysis suggests that there is an economic incentive for the construction of the benzyl acetate plant, it is important to be cognizant of any next steps that would be required. First, it is necessary to ensure that the required \$3.5 million in total capital investment is currently available for this project. While taking out a partial loan for this capital has the potential to remain a profitable option, especially in the current low interest rate environment, we recommend not proceeding with the plant's construction if that is the case. Assuming the capital has been secured, we recommend ensuring that the plant's construction is realistic within the facility and that its arrangement is advantageous in relation to the current process.

For safety, a brief risk analysis of the plant determined that the main hazards of the plant are within acceptable risk level if mitigated by safety devices, such as alarms and relief valves. A full hazard and operability (HAZOP) study was performed on the reactor as it was considered the unit with the most risk. However, before continuing with the construction of the plant, we recommend performing a full HAZOP analysis on each unit within the plant to identify any other potential safety risks. Additionally, we recommend performing fault trees for the complete draining of ST-200 and the overfilling of ST-103 in the case of equipment failure or operator negligence. Fault trees would provide insight into the frequency and probability of these incidents occurring.

Before purchasing any equipment, we recommend having an organized way of tracking all the capital purchases of the plant to ensure that the manufacturer information and part specifications are not lost over time. To further improve the organization, we recommend ensuring

a management of change (MOC) system is in place to document any changes that may occur over the twenty-year life of the plant. An organized assessment of any changes will lower the chance that a safety, environmental, or financial incident occurs. Lastly, before proceeding to implementation, we recommend closely investigating the legal requirements of operating the plant, including the acquisition of certification from the Occupational Safety and Health Administration (OSHA) and other government agencies, such as the EPA. Ultimately, these considerations will provide insight into the feasibility of moving forward with the proposed design.

PROCESS FLOW DIAGRAM AND MATERIAL BALANCES

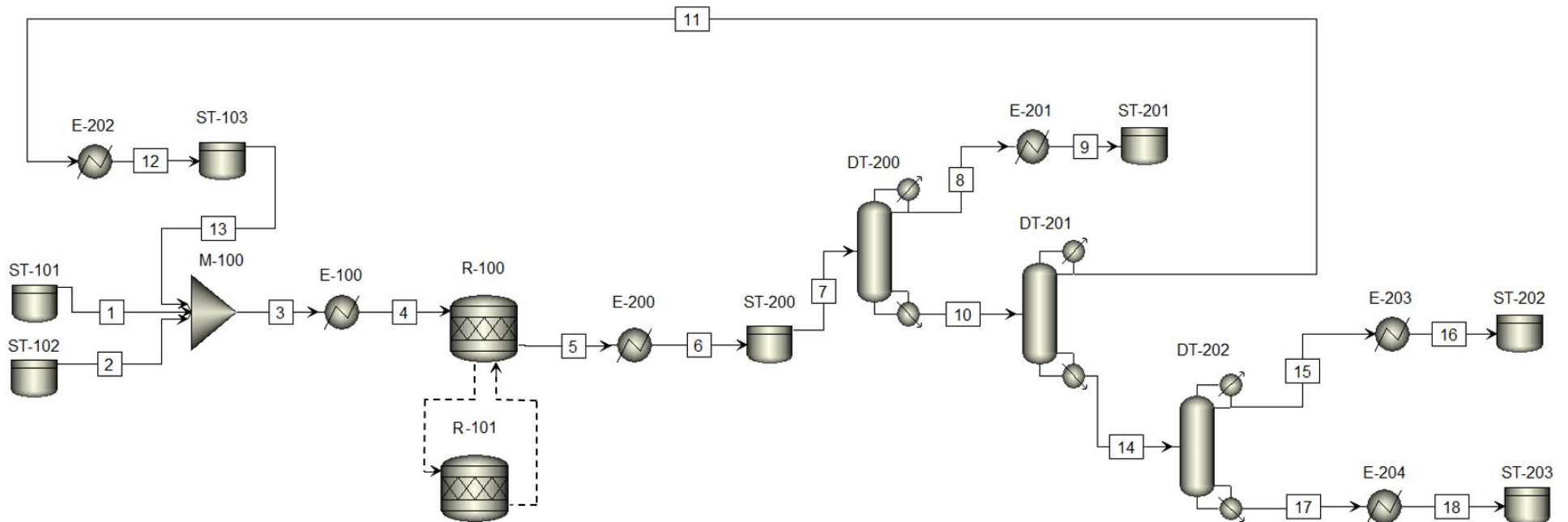


Figure 1. Process Flow Diagram (P-100 not shown but used to load/unload R-100)

Table XVI(b). Mass Balance for Components in the Feed Streams and Around the Reactor

Stream Name			1		2		3		4		5		
Phase			Liquid		Liquid		Liquid		Liquid		Liquid		
Temperature			°C	25.0	25.0	25.1	120	120					
Pressure			kPa	101.3	101.3	101.3	101.3	101.3					
Enthalpy Flow			KJ/hr	-1.70x10 ⁵	-4.76x10 ⁵	-1.16x10 ⁶	-1.06x10 ⁶	-1.10x10 ⁶					
Molecular Weight				108	60.1	98.5	98.5	98.5					
Molar Vapor Weight Fraction				-	-	-	-	-					
Molar Liquid Weight Fraction				1.00	1.00	1.00	1.00	1.00					
Total Mole Flow Rate			kmol/hr	1.09	0.986	5.24	5.24	5.24					
Total Mole Comp. Rates/Mole Fractions													
Acetic Acid			kmol/hr %	-	-	0.986	100%	1.05	20.0%	1.05	20.0%	6.23x10 ⁻²	1.2%
Benzyl Alcohol			kmol/hr %	1.09	100%	-	-	4.18	79.8%	4.18	79.8%	3.10	59.2%
Benzyl Acetate			kmol/hr %	-	-	-	-	6.70x10 ⁻³	0.1%	6.70x10 ⁻³	0.1%	0.986	18.8%
Water			kmol/hr %	-	-	-	-	7.41x10 ⁻³	0.1%	7.41x10 ⁻³	0.1%	1.04	19.8%
Dibenzyl Ether			kmol/hr %	-	-	-	-	-	-	-	-	5.19x10 ⁻²	1.0%
Total Mass Flow Rate			kg/hr	118	59.2	516	516	516					
Total Mass Comp. Rates/Mass Fractions													
Acetic Acid			kg/hr %	-	-	59.2	100%	62.9	12.2%	62.9	12.2%	3.74	0.7%
Benzyl Alcohol			kg/hr %	118	100%	-	-	452	87.6%	452	87.6%	336	65.0%
Benzyl Acetate			kg/hr %	-	-	-	-	1.01	0.19%	1.01	0.19%	148	28.7%
Water			kg/hr %	-	-	-	-	0.133	0.03%	0.133	0.03%	18.7	3.6%
Dibenzyl Ether			kg/hr %	-	-	-	-	-	-	-	-	10.3	2.0%
Total Volumetric Flow Rate			L/hr	113	55.2	485	530	534					

Table XVI(c). Mass balance for components after the reactor (R-100) and the first distillation column (DT-200)

Stream Name		6	7	8	9
Phase		Liquid	Liquid	Liquid	Liquid
Temperature		°C	25.0	25.0	100
Pressure		kPa	101.3	101.3	101.3
Enthalpy Flow		KJ/hr	-1.22x10 ⁶	-1.22x10 ⁶	-2.90x10 ⁵
Molecular Weight			98.5	98.5	18.6
Molar Vapor Weight Fraction			-	-	-
Molar Liquid Weight Fraction			1.00	1.00	1.00
Total Mole Flow Rate		kmol/hr	5.24	5.24	1.04
Total Mole Comp. Rates/Mole Fractions					
Acetic Acid		kmol/hr %	6.23x10 ⁻² 1.2%	6.23x10 ⁻² 1.2%	1.41x10 ⁻³ 0.1%
Benzyl Alcohol		kmol/hr %	3.10 59.2%	3.10 59.2%	6.00x10 ⁻³ 0.6%
Benzyl Acetate		kmol/hr %	0.986 18.8%	0.986 18.8%	- -
Water		kmol/hr %	1.04 19.8%	1.04 19.8%	1.03 99.3%
Dibenzyl Ether		kmol/hr %	5.19x10 ⁻² 1.0%	5.19x10 ⁻² 1.0%	- -
Total Mass Flow Rate		kg/hr	516	516	19.3
Total Mass Comp. Rates/Mass Fractions					
Acetic Acid		kg/hr %	3.74 0.7%	3.74 0.7%	8.50x10 ⁻² 0.4%
Benzyl Alcohol		kg/hr %	336 65.0%	336 65.0%	0.648 3.4%
Benzyl Acetate		kg/hr %	148 28.7%	148 28.7%	- -
Water		kg/hr %	18.7 3.6%	18.7 3.6%	18.6 96.2%
Dibenzyl Ether		kg/hr %	10.3 2.0%	10.3 2.0%	- -
Total Volumetric Flow Rate		L/hr	490	490	21.0

Table XVI(d). Mass balance for components around the second distillation column (DT-201)

Stream Name		10	11	12	13
Phase		Liquid	Liquid	Liquid	Liquid
Temperature		°C	200	195	25.0
Pressure		kPa	101.3	101.3	101.3
Enthalpy Flow		KJ/hr	-6.88x10 ⁵	-3.90x10 ⁵	-5.16x10 ⁵
Molecular Weight			118	107	107
Molar Vapor Weight Fraction			-	-	-
Molar Liquid Weight Fraction			1.00	1.00	1.00
Total Mole Flow Rate		kmol/hr	4.20	3.17	3.17
<i>Total Mole Comp. Rates/Mole Fractions</i>					
Acetic Acid	kmol/hr %	6.09x10 ⁻²	1.4%	6.09x10 ⁻²	1.9%
Benzyl Alcohol	kmol/hr %	3.10	73.7%	3.09	97.6%
Benzyl Acetate	kmol/hr %	0.986	23.5%	6.70x10 ⁻³	0.2%
Water	kmol/hr %	7.41x10 ⁻³	0.2%	7.41x10 ⁻³	0.2%
Dibenzyl Ether	kmol/hr %	5.19x10 ⁻²	1.2%	-	-
Total Mass Flow Rate		kg/hr	497	339	339
<i>Total Mass Comp. Rates/Mass Fractions</i>					
Acetic Acid	kg/hr %	3.66	0.7%	3.66	1.1%
Benzyl Alcohol	kg/hr %	335	67.4%	334	98.6%
Benzyl Acetate	kg/hr %	148	29.8%	1.01	0.3%
Water	kg/hr %	0.133	0.03%	0.133	0.04%
Dibenzyl Ether	kg/hr %	10.3	2.1%	-	-
Total Volumetric Flow Rate		L/hr	562	382	324

Table XVI(e). Mass balance for components around the third distillation column (DT-202)

Stream Name			14		15		16		17		18	
Phase			Liquid		Liquid		Liquid		Liquid		Liquid	
Temperature			°C	216		214		25.0		287		25.0
Pressure			kPa	101.3		101.3		101.3		101.3		101.3
Enthalpy Flow			KJ/hr	-3.09x10 ⁵		-3.10x10 ⁵		-3.62x10 ⁵		-2.10x10 ³		-3.11x10 ³
Molecular Weight				152		150		150		198		198
Molar Vapor Weight Fraction				-		-		-		-		-
Molar Liquid Weight Fraction				1.00		1.00		1.00		1.00		1.00
Total Mole Flow Rate			kmol/hr	1.04		0.986		0.986		0.0519		0.0519
Total Mole Comp. Rates/Mole Fractions												
Acetic Acid			kmol/hr %	-	-	-	-	-	-	-	-	-
Benzyl Alcohol			kmol/hr %	6.70x10 ⁻³	0.6%	6.70x10 ⁻³	0.7%	6.70x10 ⁻³	0.7%	-	-	-
Benzyl Acetate			kmol/hr %	0.979	94.4%	0.979	99.3%	0.979	99.3%	3.13x10 ⁻⁴	0.6%	3.13x10 ⁻⁴
Water			kmol/hr %	-	-	-	-	-	-	-	-	-
Dibenzyl Ether			kmol/hr %	5.19x10 ⁻²	5.0%	3.14x10 ⁻⁴	0.03%	3.14x10 ⁻⁴	0.03%	5.16x10 ⁻²	99.5%	5.16x10 ⁻²
Total Mass Flow Rate			kg/hr	158		148		148		10.3		10.3
Total Mass Comp. Rates/Mass Fractions												
Acetic Acid			kg/hr %	-	-	-	-	-	-	-	-	-
Benzyl Alcohol			kg/hr %	0.725	0.5%	0.725	0.5%	0.725	0.5%	-	-	-
Benzyl Acetate			kg/hr %	147	93.0%	147	99.5%	147	99.5%	4.70x10 ⁻²	0.5%	4.70x10 ⁻²
Water			kg/hr %	-	-	-	-	-	-	-	-	-
Dibenzyl Ether			kg/hr %	10.3	6.5%	6.22x10 ⁻²	0.04%	6.22x10 ⁻²	0.04%	10.2	99.5%	10.2
Total Volumetric Flow Rate			L/hr	183		171		141		12.6		9.87

REFERENCES

1. Benhmid, A., et al., *Direct synthesis of benzyl acetate and optimization of reaction conditions for the gas phase acetoxylation of toluene*, Volume 112, Issues 1-4, March 2006, p. 192-196. https://www.researchgate.net/publication/244322101_Direct_synthesis_of_benzyl_acetate_and_optimisation_of_reaction_conditions_for_the_gas_phase_acetoxylation_of_toluene Abdelhadi (Accessed March 1, 2020).
2. Madaan, N; Gatla, S; Kalevaru, V; Radnik, J; Pohl, M; Lucke, B; Bruckner, A; Martin, A; "The Impact of Reaction Pressure on the Catalytic Performance of the Pd-Sb/TiO₂ Catalyst in the Acetoxylation of *Toluene into Benzyl Acetate*", Published 26 October, 2012. <https://onlinelibrary.wiley.com/doi/full/10.1002/cctc.201200522> (Accessed March 1, 2020).
3. Melo, A.D.Q., et al., *Synthesis of Benzyl Acetate Catalyzed by Lipase Immobilized in Nontoxic Chitosan-Polyphosphate Beads*. *Molecules*, 2017. 22(12).
4. Acetaldehyde; MSDS No. S25115[Online]; Global Safety Management Inc, Feb 10, 2015. https://betastatic.fishersci.com/content/dam/fishersci/en_US/documents/programs/education/regulatory-documents/sds/chemicals/chemicals-a/S25115.pdf (accessed January 30, 2020).
5. "Material Safety Data Sheet – Vinyl Acetate" <https://www.fishersci.com/shop/msdsproxy?productName=O50574&productDescrip>, ThermoFisher Scientific, 2019 (accessed March 4, 2020).
6. "Material Safety Data Sheet - Acetic acid". https://betastatic.fishersci.com/content/dam/fishersci/en_US/documents/programs/education/regulatory-documents/sds/chemicals/chemicals-a/S25118.pdf, ThermoFisher Scientific, 2015 (accessed March 4, 2020).
7. "Material Safety Data Sheet – Benzyl Alcohol" https://betastatic.fishersci.com/content/dam/fishersci/en_US/documents/programs/education/regulatory-documents/sds/chemicals/chemicals-b/S25666A.pdf, ThermoFisher Scientific, 2019 (accessed March 4, 2020).
8. "Material Safety Data Sheet – Benzyl Acetate" Fisher Scientific. <https://fscimage.fishersci.com/msds/02775.htm> (accessed March 4, 2020).
9. "Material Safety Data Sheet - Dibenzyl Ether" <https://www.sigmaaldrich.com/catalog/product/sial/33630?lang=en®ion=US>, Sigma-Aldrich, 2020 (accessed March 4, 2020).
10. "Rule 391-3-6-.03. Water Use Classifications and Water Quality Standards", United States Environmental Protection Agency, 2016. <https://www.epa.gov/sites/production/files/2014-12/documents/gawqs.pdf> (Accessed April 9, 2020)
11. "Title 40: Protection of Environment, PART 711—TSCA CHEMICAL DATA REPORTING REQUIREMENTS", Code of Federal Regulations (CFR), 2020. https://www.ecfr.gov/cgi-bin/text-idx?SID=d0ff709a0e84960f6ea05bedf81e4370&node=pt40.31.711&rgn=div5#se40.33.711_11 (Accessed April 9, 2020)
12. "Initial List of Hazardous Air Pollutants with Modifications", United States Environmental Protection Agency. <https://www.epa.gov/haps/initial-list-hazardous-air-pollutants-modifications> (Accessed April 9, 2020)

13. Nandiwale, K.Y., et al., *Benzylation of acetic acid to benzyl acetate over highly active and reusable Micro/Meso-HZSM-5*. Chemical Engineering Research & Design, 2015. p. 584-590.
14. Tschentscher, R., et al., *Liquid-Solid Mass Transfer in Agitated Slurry Reactors and Rotating Solid Foam Reactors*. Ind.Eng.Chem.Res. 2010, 49, 10758-10766
15. Fogler, S. “*Elements of Chemical Reaction Engineering*”, Prentice Hall 2016, Fifth Edition. pp. 348-356.
16. ZSM-5 Zeolite, Millipore Sigma.
<https://www.sigmaaldrich.com/catalog/product/sigma/96096?lang=en®ion=US>
(Accessed March 15, 2020)
17. Cordero-Lanzac, T; Ateka, A; Uriart-Perez, P; Castanho, P; Aguayo, A; Bilbao, J. “*Insight into the Deactivation and Regeneration of HZSM-5 Zeolite Catalysts in the Conversion of Dimethyl Ether to Olefins*”. *Industrial and Engineering Chemical Research*, July, 2018.
<https://pubs.acs.org/doi/pdf/10.1021/acs.iecr.8b03308> (Accessed March 1, 2020).
18. Standard Pumps for Drums and Totes. <https://www.carotek.com/Product/Standard-Pumps-for-Drums-and-Totes> (Accessed April 3, 2020)
19. Seider, W; Lewin, D; Seader, JD; Widagdo, S; Gani, R; Ng, K; “*Product and Process Design Principles; Synthesis Analysis and Evaluation*”, Wiley, Fourth Edition. Pp. 498-510.
20. 275 Gallon Reconditioned IBC Tote Tank, National Tank Outlet.
<https://www.ntotank.com/275gallon-nto-white-ibc-new-tote-tank-x2008473> (Accessed April 1, 2020)
21. Crowl, D; Louvar, Joseph; “*Chemical Process Safety: Fundamentals with Applications*”, Prentice Hall 2011, Third Edition.
22. Zeolite; MSDS No. ZSM-5 [Online]; Global Safety Management Inc, Jan 19,2018.
<https://www.fishersci.com/store/msds?partNumber=AC279571000&productDescription=ZEOLITE+WITHOUT+ALUMINUM+100G&vendorId=VN00032119&countryCode=US&language=en> (accessed January 30, 2020).
23. “*Control Techniques for Volatile Organic Compound Emissions from Stationary Sources*”, United States Environmental Protection Agency, 1992
24. Mitra. S; “*Design Considerations of hot oil system*”, Research Gate, 2015
https://www.researchgate.net/publication/279298058_A_techincal_report_on_design_of_hot_oil_system (Accessed April 5, 2020)
25. Mohamed A. Fahim; Taher A. Alsahhaf; Amal Elkilani., “*Fundamentals of Petroleum Refining*”, 2010, Pp. 357-376
26. “*Resource Conservation and Recovery Act (RCRA) and Federal Facilities*”, United States Environmental Protection Agency, 1986. <https://www.epa.gov/enforcement/resource-conservation-and-recovery-act-rcra-and-federal-facilities> (Accessed April 9, 2020)
27. Dibenzyl Ether, Millipore Sigma.
<https://www.sigmaaldrich.com/catalog/product/aldrich/108014?lang=en®ion=US>
(Accessed April 1, 2020)
28. Smith, J.M; Van Ness, H. C.;Abbott, M. M.;Swihart, M. T; “*Introduction to Chemical Engineering Thermodynamics*”, Mc Graw Hill Education, Eighth edition. Pp. 684-686.

APPENDIX A: KINETICS/TRANSPORT CALCULATIONS

A-1. Method for Determining Kinetic Constants

The following conversion data was first plotted below to determine the rate constants at various temperatures.¹³

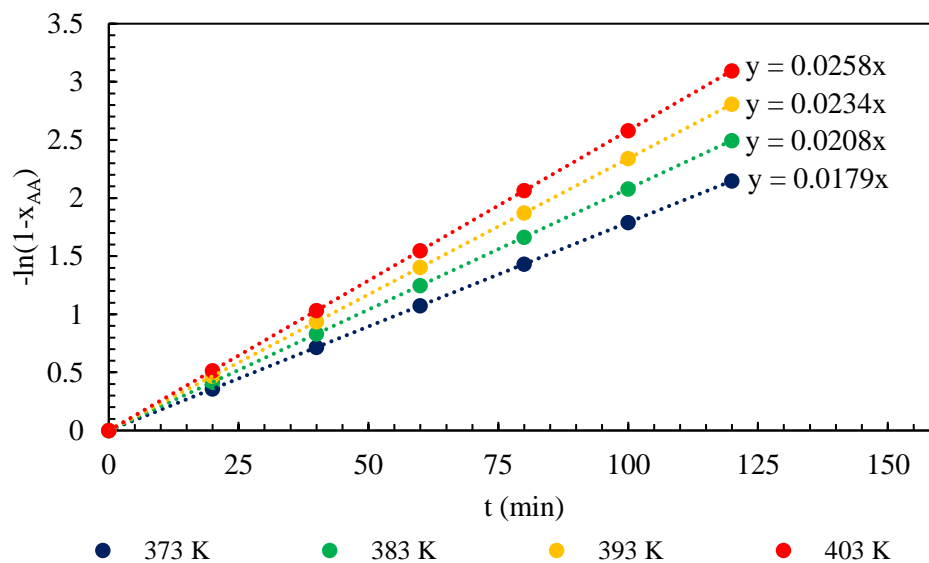


Figure A1. Chemical Route Conversion Data to Determine Rate Constants

The linearized Arrhenius plot below is then used to determine E_a and A .¹³

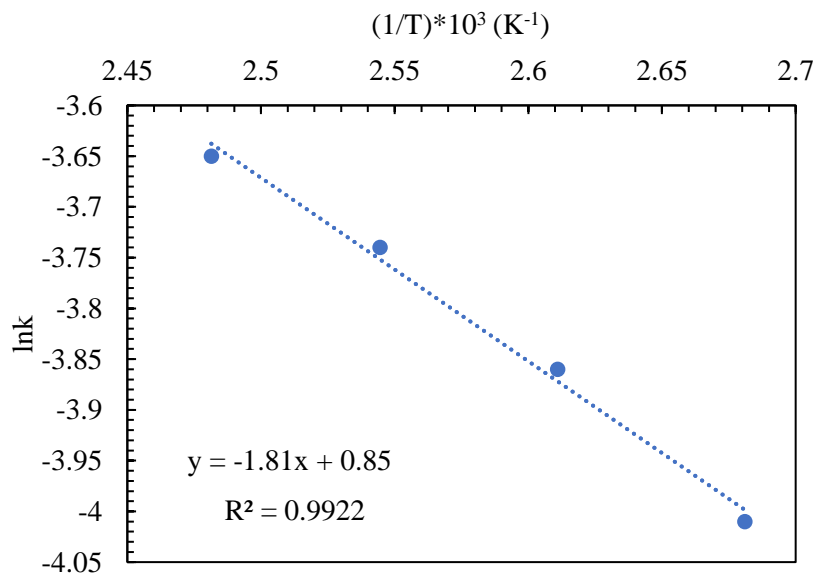


Figure A2. Chemical Route Linearized Arrhenius Plot

Using the determined E_a (15.07 kJ/mol) and A (2.34 min^{-1}), the temperature of the reactor was chosen to be 393K. While this decision was determined from the data presented in Nandiwale, this temperature is a reasonable choice because a high conversion can be achieved (94%).¹³ The rate of increase in conversion decreases beyond 393K.

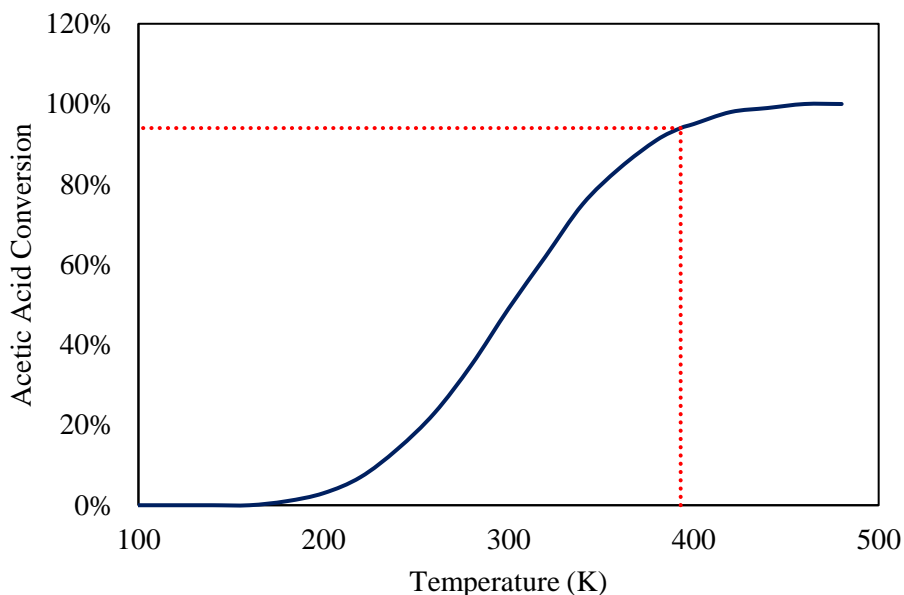


Figure A3. Conversion Achieved in Two Hours at Various Temperatures

A-2. Method for Determining Rate

The equations below were used to calculate the instantaneous rate:

$$r = Ae^{-E_a/RT} [CH_3COOH]$$

$$r = 2.34e^{(-15070J/mol)/(8.314\frac{J}{molK})(393K)} [CH_3COOH]$$

$$r = 0.023[CH_3COOH]$$

This rate varies with concentration, so the reaction was discretized into rate by the minute, shown in the table below. The following initial starting values were used per batch: 12,576 mol benzyl alcohol, 3,144 mol acetic acid, 0 mol dibenzyl ether, 0 mol benzyl acetate, and 0 mol water. After 6 iterations of using the output flows from Microsoft Excel (2019) and the recycled inlet flows from ASPEN, the final values were determined. The sixth iteration is shown in the table below.

Table AI. Chemical Route Kinetics Showing Conversion Over Time

Time (min)	Moles of AA (mol)	Change in Moles (mol)	% Conversion
0	3144.0	73.1	0%
1	3070.9	71.4	2%
2	2999.5	69.7	5%
3	2929.7	68.1	7%
4	2861.6	66.5	9%
5	2795.1	65.0	11%
6	2730.1	63.5	13%
7	2666.6	62.0	15%
8	2604.6	60.6	17%
9	2544.0	59.2	19%
10	2484.9	57.8	21%
11	2427.1	56.4	23%
12	2370.7	55.1	25%
13	2315.5	53.8	26%
14	2261.7	52.6	28%
15	2209.1	51.4	30%
16	2157.7	50.2	31%
17	2107.6	49.0	33%
18	2058.6	47.9	35%
19	2010.7	46.8	36%
20	1963.9	45.7	38%
21	1918.3	44.6	39%
22	1873.7	43.6	40%
23	1830.1	42.6	42%
24	1787.6	41.6	43%
25	1746.0	40.6	44%
26	1705.4	39.7	46%
27	1665.7	38.7	47%
28	1627.0	37.8	48%
29	1589.2	37.0	49%
30	1552.2	36.1	51%
31	1516.1	35.3	52%
32	1480.9	34.4	53%
33	1446.4	33.6	54%
34	1412.8	32.9	55%
35	1380.0	32.1	56%
36	1347.9	31.3	57%
37	1316.5	30.6	58%
38	1285.9	29.9	59%
39	1256.0	29.2	60%

40	1226.8	28.5	61%
41	1198.3	27.9	62%
42	1170.4	27.2	63%
43	1143.2	26.6	64%
44	1116.6	26.0	64%
45	1090.7	25.4	65%
46	1065.3	24.8	66%
47	1040.5	24.2	67%
48	1016.3	23.6	68%
49	992.7	23.1	68%
50	969.6	22.5	69%
51	947.1	22.0	70%
52	925.1	21.5	71%
53	903.5	21.0	71%
54	882.5	20.5	72%
55	862.0	20.0	73%
56	842.0	19.6	73%
57	822.4	19.1	74%
58	803.3	18.7	74%
59	784.6	18.2	75%
60	766.3	17.8	76%
61	748.5	17.4	76%
62	731.1	17.0	77%
63	714.1	16.6	77%
64	697.5	16.2	78%
65	681.3	15.8	78%
66	665.5	15.5	79%
67	650.0	15.1	79%
68	634.9	14.8	80%
69	620.1	14.4	80%
70	605.7	14.1	81%
71	591.6	13.8	81%
72	577.8	13.4	82%
73	564.4	13.1	82%
74	551.3	12.8	82%
75	538.5	12.5	83%
76	525.9	12.2	83%
77	513.7	11.9	84%
78	501.8	11.7	84%
79	490.1	11.4	84%
80	478.7	11.1	85%
81	467.6	10.9	85%
82	456.7	10.6	85%

83	446.1	10.4	86%
84	435.7	10.1	86%
85	425.6	9.9	86%
86	415.7	9.7	87%
87	406.0	9.4	87%
88	396.6	9.2	87%
89	387.4	9.0	88%
90	378.4	8.8	88%
91	369.6	8.6	88%
92	361.0	8.4	89%
93	352.6	8.2	89%
94	344.4	8.0	89%
95	336.4	7.8	89%
96	328.5	7.6	90%
97	320.9	7.5	90%
98	313.4	7.3	90%
99	306.2	7.1	90%
100	299.0	7.0	90%
101	292.1	6.8	91%
102	285.3	6.6	91%
103	278.7	6.5	91%
104	272.2	6.3	91%
105	265.8	6.2	92%
106	259.7	6.0	92%
107	253.6	5.9	92%
108	247.7	5.8	92%
109	242.0	5.6	92%
110	236.3	5.5	92%
111	230.8	5.4	93%
112	225.5	5.2	93%
113	220.2	5.1	93%
114	215.1	5.0	93%
115	210.1	4.9	93%
116	205.2	4.8	93%
117	200.5	4.7	94%
118	195.8	4.6	94%
119	191.2	4.4	94%
120	186.8		94%

A-3. Transport Effect Calculations

A stirring rate of 200 rpm and a power output of $100 \frac{W}{m^3}$ were used based on the mass transfer coefficient (k_L) values of 0.15 cm/s presented in Figures 4 and 10 from Tschentcher.¹⁴ Using a particle size of 1.5 micron, Da is calculated to be than 0.1.

$$\begin{aligned} \text{no. of particles of catalyst} &= \frac{\text{mass of catalyst}}{\text{density of catalyst}} * \frac{1}{\text{total surface area}} \\ &= \frac{18.8 \text{ kg of catalyst}}{850 \frac{\text{kg}}{\text{m}^3}} * \frac{1}{4/3 * \pi * r^3} = 4.64 \times 10^{11} \end{aligned}$$

$$-r_a = \frac{-r_a}{(\text{reaction medium})} = \frac{0.508 \frac{\text{mol}}{\text{s}}}{1508 \text{ L}} = 3.37 \times 10^{-4} \frac{\text{mol}}{\text{s} * \text{L}}$$

$$[Ca]_{\text{bulk}} = \frac{\text{mol of substrate (limiting reactant)}}{\text{total volume}} = \frac{3330 \text{ mol}}{1.58 \text{ m}^3} = 2102.27 \frac{\text{mol}}{\text{m}^3}$$

$$\begin{aligned} a &= \frac{\text{no. of particles} * \text{particle surface area}}{\text{total volume}} = \frac{4.64 \times 10^{11} * 4 * \pi * r^2}{1508 \text{ L}} \\ &= 2.17 \times 10^{-3} \frac{\text{m}^2}{\text{L}} \end{aligned}$$

$$Da = \frac{-r_a}{k_L * a * [Ca]_{\text{bulk}}} = \frac{3.37 \times 10^{-4} \frac{\text{mol}}{\text{s} * \text{L}}}{0.0015 \frac{\text{m}}{\text{s}} * 2.17 \times 10^{-3} \frac{\text{m}^2}{\text{L}} * 2102.27 \frac{\text{mol}}{\text{m}^3}} = \mathbf{0.0491} < \mathbf{0.1}$$

APPENDIX B: TERNARY PHASE DIAGRAMS

B-1. Ternary Diagram of Water/Benzyl Alcohol/Benzyl Acetate

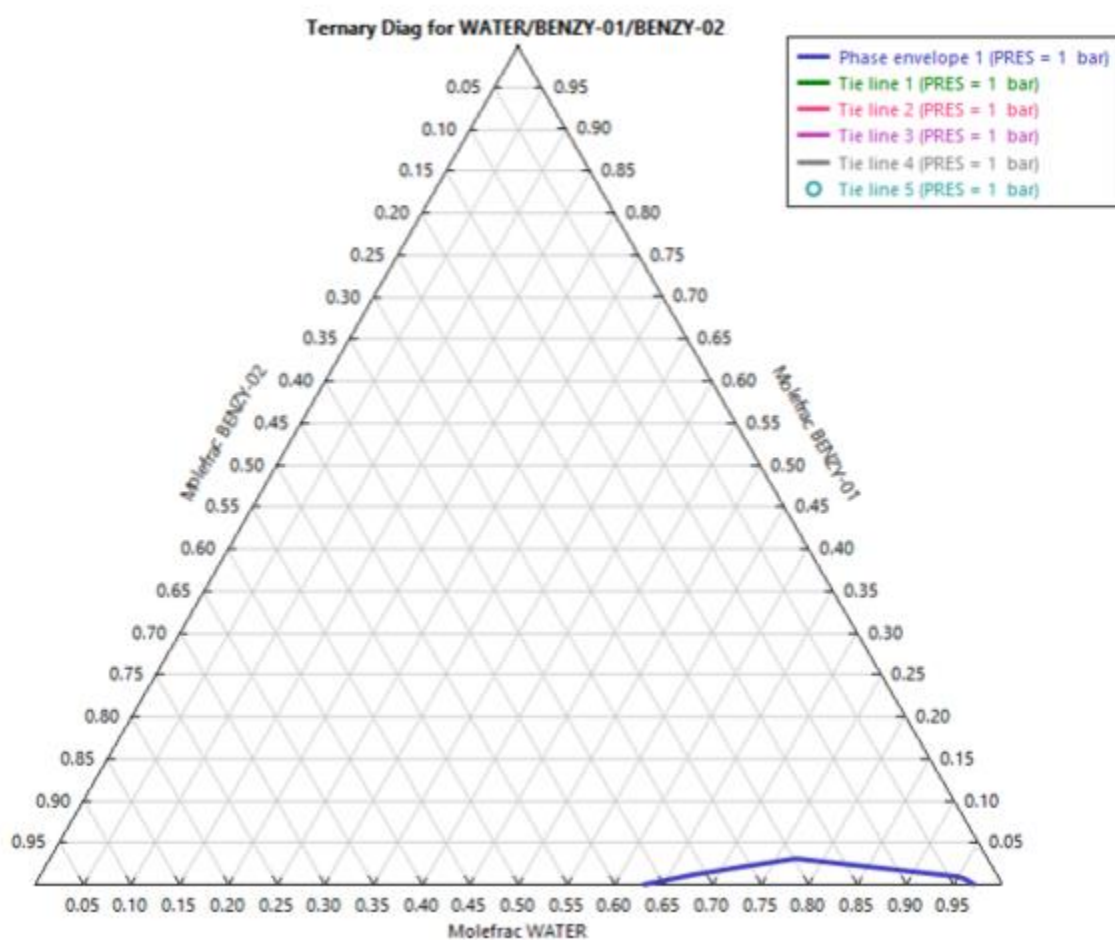


Figure B1. Ternary Diagram of Water/Benzyl Alcohol/Benzyl Acetate

B-2. Ternary Diagram of Water/Dibenzyl Ether/Benzyl Alcohol

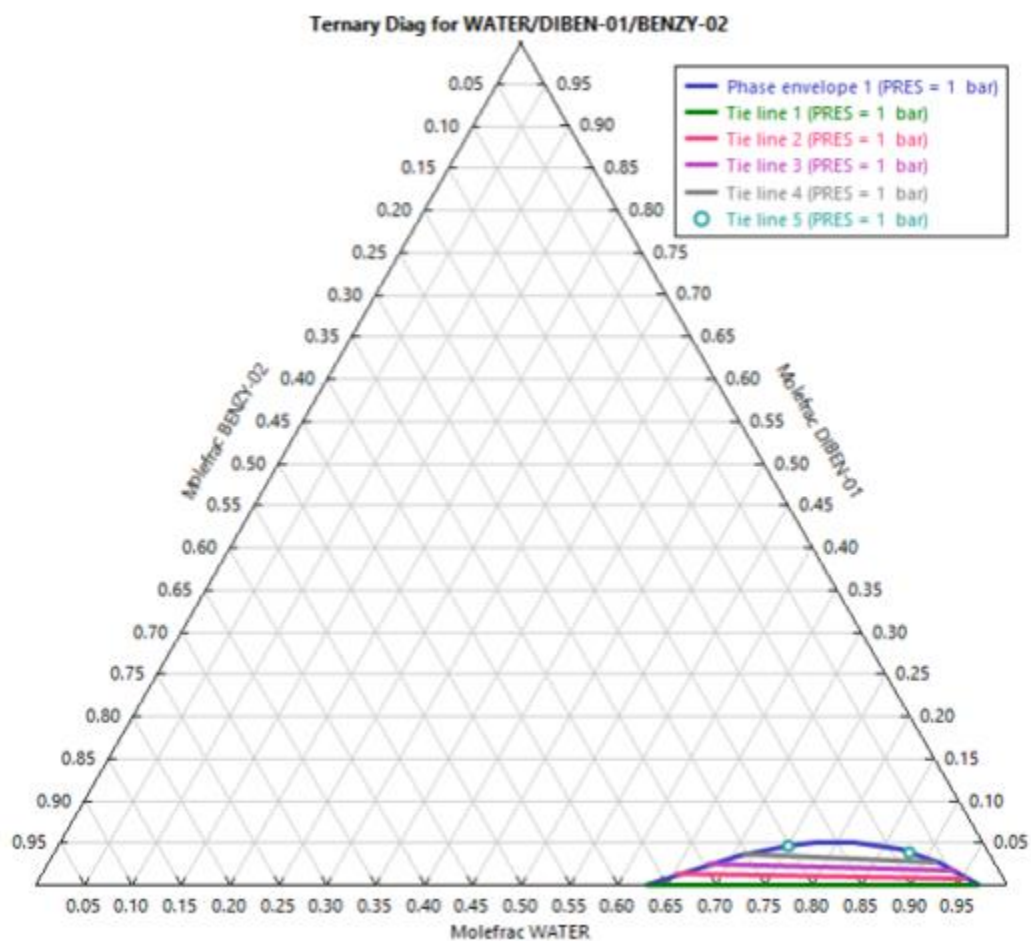


Figure B2. Ternary Diagram of Water/Dibenzyl Ether/Benzyl Alcohol

APPENDIX C: ENERGY/UTILITY SAMPLE CALCULATIONS

C-1. Heat of Reaction Calculation

Table CI. Enthalpies and Heat Capacities of Chemical Route Components at 298 K²⁸

Component	Enthalpy (J/mol)	C _p (J/mol K)
Acetic Acid	-484,500	123.1
Benzyl Alcohol	-167,000	215.9
Benzyl Acetate	-309,150	148.5
Water	-292,740	75.3
Dibenzyl Ether	19,299	294.1

The chemical reaction occurs at 393 K, so enthalpies are adjusted from 298 K to 393 K using the following equation:

$$\Delta H_{rxn}(T_2) = \Delta H_{rxn}(T_1) + \int_{T_1}^{T_2} \Delta C_p \Delta T$$

Table CII. Enthalpies of Chemical Route Components at 393 K

Component	Enthalpy (J/mol)
Acetic Acid	-472,806
Benzyl Alcohol	-146,486
Benzyl Acetate	-295,043
Water	-285,587
Dibenzyl Ether	47,240

Reactions Occurring:

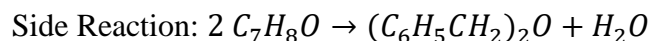
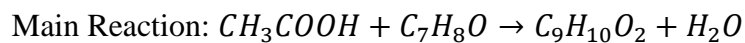
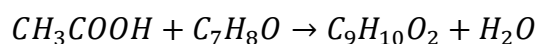


Table CIII. Moles of Components per Batch with Benzyl Alcohol Fed in Excess

Component	n_{in}	n_{out}	Δn_{total}	Δn_{main}	Δn_{side}
Acetic Acid	3,144	187	-2,958	-2,957	-
Benzyl Alcohol	12,576	9,308	-3,264	-2,957	-311
Benzyl Acetate	-	2,957	2,957	2,957	-
Water	-	3,113	3,113	2,957	156
Dibenzyl Ether	-	156	156	-	156

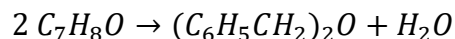
$$\text{Heat of Reaction} = \Delta H_{rxn} = \sum v \cdot n \cdot \Delta H_f(\text{products}) - \sum v \cdot n \cdot \Delta H_f(\text{reactants})$$

For the Main Reaction:



$$\Delta H_{rxn} = \left[\left(1 * 2957 \text{ mol} * -295.04 \frac{\text{kJ}}{\text{mol}} \right) + \left(1 * 2957 \text{ mol} * -285.59 \frac{\text{kJ}}{\text{mol}} \right) \right] - \left[\left(1 * 2957 \text{ mol} * -146.49 \frac{\text{kJ}}{\text{mol}} \right) + \left(1 * 2957 \text{ mol} * -472.81 \frac{\text{kJ}}{\text{mol}} \right) \right] = \mathbf{114,332 \text{ kJ}}$$

For the Side Reaction:



$$\Delta H_{rxn} = \left[\left(1 * 155.6 \text{ mol} * -47.24 \frac{\text{kJ}}{\text{mol}} \right) + \left(1 * 155.6 \text{ mol} * -285.59 \frac{\text{kJ}}{\text{mol}} \right) \right] - \left[\left(2 * 311 \text{ mol} * -146.49 \frac{\text{kJ}}{\text{mol}} \right) \right] = \mathbf{54,100 \text{ kJ}}$$

Total Heat of Reaction:

$$\Delta H_{rxn}^0 = \frac{114,332 \text{ kJ} + 54,100 \text{ kJ}}{2 \text{ hr for reaction}} = \mathbf{84,216 \text{ kJ/hr}}$$

C-2. Utility Costs Calculations

Table CIV. Utility Costs¹⁹

Utility	Cost	Units
Electricity	\$0.07	kWh
Natural Gas (to Heat Hot Silicon Oil)	\$4	MMBtu
Wastewater Treatment	\$0.45	gallon
Solid Waste	\$150	ton
Chilled Water	\$1.50	ton-day

Electricity Cost:

$$\begin{aligned}
 & \text{Net Power} \left(\frac{kJ}{hr} \right) * \frac{1 \text{ kWh}}{3600 \text{ kJ}} * \frac{\text{Batch Operating hrs}}{\text{year}} * \frac{\text{Price}}{\text{kWh}} \\
 & 1.16 * 10^4 \frac{kJ}{hr} * \frac{1 \text{ kWh}}{3600 \text{ kJ}} * \frac{2700 \text{ hrs}}{\text{year}} * \frac{\$0.07}{\text{kWh}} = \mathbf{\$607/\text{year}}
 \end{aligned}$$

Heating Cost (Hot Oil/Natural Gas):

$$\begin{aligned}
 & \left(\frac{\text{Heat Duty} \frac{kJ}{hr}}{0.85} \right) * \frac{3412 \text{ BTU}}{3600 \frac{kJ}{hr}} * \frac{\text{Operating hrs}}{\text{Year}} * \frac{1 \text{ BTU}}{1,000,000 \text{ BTU}} * \left(\frac{\text{Price}}{\text{MMBTU}} \right) \\
 & \left(\frac{1.26 * 10^5 \frac{kJ}{hr}}{0.85} \right) * \frac{3412 \text{ BTU}}{3600 \frac{kJ}{hr}} * \frac{4700 \text{ hrs}}{\text{Year}} * \frac{1 \text{ BTU}}{1,000,000 \text{ BTU}} * \left(\frac{\$4}{\text{MMBTU}} \right) = \mathbf{\$2,917/\text{year}}
 \end{aligned}$$

Wastewater Treatment Cost:

$$\begin{aligned}
 & \text{Stream vol. flowrate} * \frac{\text{Continuous op. hours}}{\text{year}} * \frac{\text{Price of treatment}}{\text{gal}} \\
 & \left(12.4 \frac{L}{hr} \right) * \frac{1 \text{ gal}}{3.785 \text{ L}} * \frac{4700 \text{ hrs}}{1 \text{ year}} * \frac{\$0.45}{\text{gal}} = \mathbf{\$6,929/\text{year}}
 \end{aligned}$$

Solid Waste (Catalyst):

$$\begin{aligned}
 & \text{Disposal Rate} \left(\frac{kg}{yr} \right) * \frac{1 \text{ ton}}{907.185 \text{ kg}} * \frac{\$150}{\text{ton}} \\
 & 1,132.8 \text{ kg/yr} * \frac{1 \text{ ton}}{907.185 \text{ kg}} * \frac{\$150}{\text{ton}} = \mathbf{\$190/\text{year}}
 \end{aligned}$$

Cooling Cost (Chilled Water):

$$\text{Heat Duty } \left(\frac{\text{kJ}}{\text{hr}} \right) * \frac{3412 \text{ BTU}}{3600 \frac{\text{kJ}}{\text{hr}}} * \frac{1 \text{ ton-day}}{288,000 \text{ BTU}} * \frac{\text{Operating hrs}}{\text{year}} * \frac{\$1.5}{\text{ton-day}}$$

$$6.24 * 10^4 \frac{\text{kJ}}{\text{hr}} * \frac{3412 \text{ BTU}}{3600 \frac{\text{kJ}}{\text{hr}}} * \frac{1 \text{ ton-day}}{288,000 \text{ BTU}} * \frac{5400 \text{ hrs}}{\text{year}} * \frac{\$1.5}{\text{ton-day}} = \$ \mathbf{1,665/year}$$

C-3. Batch Energy Calculations

For the batch reactors: R-100 and R-101

The utility over a batch was found using the total heat of reaction as calculated in Appendix C-1 and multiplying it by the total reaction time.

$$\Delta H_{rxn} * \text{total reaction time}$$

$$42,108 \frac{\text{kJ}}{\text{hr}} * 2 \text{ hours} = 84,200 \frac{\text{kJ}}{\text{batch}}$$

The maximum rate was found by using the initial rate of conversion for acetic acid (see Table AI in Appendix A) and the heat of formation for acetic acid at 393 K (see Table CII in Appendix C).

$$r_{AA} * H_{f,AA}$$

$$36.6 \frac{\text{mol}}{\text{min}} * 472,806 \frac{\text{J}}{\text{mol}} = -17,282,300 \frac{\text{J}}{\text{min}}$$

$$-17,282,300 \frac{\text{J}}{\text{min}} * \frac{1 \text{ kJ}}{1000 \text{ J}} * \frac{1 \text{ min}}{60 \text{ seconds}} = -288.0 \frac{\text{kJ}}{\text{s}} = \mathbf{-288.0 \text{ kW}}$$

Other batch units: HEX, Pump, Agitator

The continuous energy value (kJ/hr) was used as a basis, and the total time for each batch was multiplied to convert to utility over a batch.

$$\text{Heat Duty } \left(\frac{\text{kJ}}{\text{hr}} \right) * \text{total batch time}$$

$$50,000 \frac{\text{kJ}}{\text{hr}} * 3 \frac{\text{hours}}{\text{batch}} = 150,000 \frac{\text{kJ}}{\text{batch}}$$

The heat exchangers were assumed to maintain a constant rate over the 3 hours required per batch. The pump was assumed to maintain a constant rate over one batch, and the agitator was assumed to maintain a constant rate over two batches. The maximum rate was found by converting the continuous energy value (kJ/hr) to kW.

$$\text{Heat Duty} \left(\frac{kJ}{hr} \right) * \frac{1 \text{ hr}}{3600 \text{ seconds}} = \frac{kJ}{s} = kW$$

$$50,000 \frac{kJ}{hr} * \frac{1 \text{ hr}}{3600 \text{ seconds}} = \mathbf{13.9 \text{ kW}}$$

APPENDIX D: HEAT INTEGRATION

D-1. Pinch Temperature Calculation

The streams considered for heat integration were taken from heat exchangers and reboilers/condensers from distillation columns. A minimum temperature of 10°C was chosen and the hot streams were adjusted as followed:

Unit		ASPEN Q		T _{in}	T _{in} (adjusted for Hot Streams)	T _{out}	T _{out} (adjusted for Hot Streams)	C
		[kJ/hr]	[kW]	[C]	[C]	[C]	[C]	[kW/C]
E-100		1.00E+05	27.81	25.09524125	25.09524125	119.85	119.85	0.294
E-200		-1.25E+05	-34.693	119.85	109.85	25	15	0.366
E-201		-5.86E+03	-1.627	100.064138	90.064138	25	15	0.022
E-202		-1.26E+05	-34.924	194.9761222	184.9761222	25	15	0.205
E-203		-5.17E+04	-14.363	213.9044838	203.9044838	25	15	0.076
E-204		-5.21E+03	-1.448	287.3061174	277.3061174	25	15	0.006
DT-200	Condenser	-8.50E+04	-23.621		100.064		99.064	23.620617
	Reboiler	3.27E+05	90.719		200.116		201.116	90.7186446
DT-201	Condenser	-1.69E+06	-470.625		194.976		193.976	470.625117
	Reboiler	1.68E+06	467.638		215.922		216.922	467.638417
DT-202	Condenser	-8.01E+04	-22.263		213.904		212.904	22.2629659
	Reboiler	8.11E+04	22.539		286.306		287.306	22.5387237

Figure D1. Heat Integration Overview

A temperature interval diagram was constructed, and the enthalpy differences between each temperature interval were calculated starting at the hottest temperature.

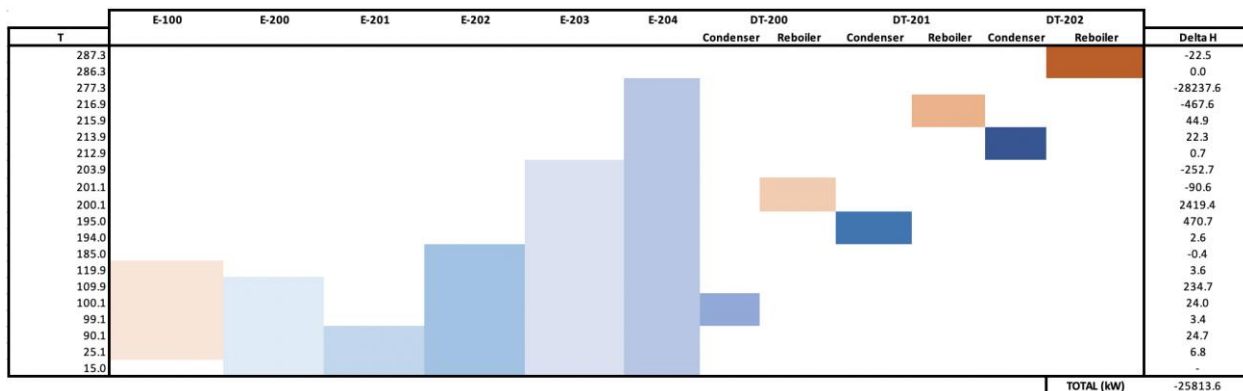


Figure D2. Temperature Interval Diagram

From there, a cascade diagram was constructed. Cascade 1 begins with a heat duty of zero. Each individual enthalpy is calculated using the previous enthalpy plus the corresponding change in enthalpy. From Cascade 1, the most negative enthalpy value is chosen. This value is made positive and is the starting enthalpy value for Cascade 2. In Cascade 2, again, each individual enthalpy is calculated using the previous enthalpy plus the corresponding change in enthalpy. From Cascade 2, the enthalpy corresponding to zero is chosen to find the cold pinch temperature.

	Cascade 1		Cascade 2		T (C)
Delta H (kW)	QH	0	QH	29003.2	287.3
-22.5	H1	-22.5	H1	28980.6	286.3
0.0	H2	-22.5	H2	28980.7	277.3
-28237.6	H3	-28260.1	H3	743.1	216.9
-467.6	H4	-28727.7	H4	275.4	215.9
44.9	H5	-28682.8	H5	320.4	213.9
22.3	H6	-28660.5	H6	342.6	212.9
0.7	H7	-28659.8	H7	343.4	203.9
-252.7	H8	-28912.5	H8	90.6	201.1
-90.6	H9	-29003.2	H9	0.0	200.1
2419.4	H10	-26583.7	H10	2419.4	195.0
470.7	H11	-26113.0	H11	2890.1	194.0
2.6	H12	-26110.4	H12	2892.7	185.0
-0.4	H13	-26110.9	H13	2892.3	119.9
3.6	H14	-26107.3	H14	2895.9	109.9
234.7	H15	-25872.6	H15	3130.6	100.1
24.0	H16	-25848.6	H16	3154.5	99.1
3.4	H17	-25845.2	H17	3158.0	90.1
24.7	H18	-25820.4	H18	3182.7	25.1
6.8	H19	-25813.6	H19	3189.5	15.0

Figure D3. Cascade Diagram

As shown above, a cold pinch temperature of 200.1°C is found for the system. Below the pinch, the heat capacity of cold streams must be less than the heat capacity of hot streams in order to heat integrate.

Unit		ASPEN Q		Tin	Tin (adjusted for Cold Streams)	Tout	Tout (adjusted for Cold Streams)	C	BELOW PINCH
		[kJ/hr]	[kW]	[C]	[C]	[C]	[C]	[kW/C]	(Cc < Ch)
E-100	C1	1.00E+05	27.81	25.09524	25.09524	119.85	119.85	0.294	0.294 < 23.6
E-200	H1	-1.25E+05	-34.693	119.85	109.85	25	15	0.366	
E-201	H2	-5.86E+03	-1.627	100.0641	90.06414	25	15	0.022	
E-202	H3	-1.26E+05	-34.924	194.9761	184.9761	25	15	0.205	
E-203	H4	-5.17E+04	-14.363	213.9045	203.9045	25	15	0.076	
E-204	H5	-5.21E+03	-1.448	287.3061	277.3061	25	15	0.006	
DT-200	Condenser	-8.50E+04	-23.621		100.064		99.064	23.62062	
	Reboiler	3.27E+05	90.719		200.116		201.116	90.71864	

Figure D4. Pinch Diagram

Above the pinch, the heat capacity of cold streams must be greater than the heat capacity of hot streams in order to heat integrate.

Unit		ASPEN Q	Tin	Tin (adjusted for Cold Streams)	Tout	Tout (adjusted for Cold Streams)	C	ABOVE PINCH
		[kJ/hr] [kW]	[C]	[C]	[C]	[C]	[kW/C]	(Cc > Ch)
DT-200	Reboiler	3.27E+05 90.719		200.116		201.116	90.71864	90.7 > 0.076
	Condenser	-1.69E+06 -470.625		194.976		193.976	470.6251	
DT-201	Reboiler	1.68E+06 467.638		215.922		216.922	467.6384	467 > 0.006
	Condenser	-8.01E+04 -22.263		213.904		212.904	22.26297	
DT-202	Reboiler	8.11E+04 22.539		286.306		287.306	22.53872	

Figure D5. Pinch Diagram (Continued)

D-2. Below the Pinch Sample Calculation

The two major energy requirements that were chosen for heat integration were the heating in E-100 and the cooling of the condenser in DT-201. The heat duty requirements and temperature values across the units were pulled from ASPEN.

Table D-2(I). Heat Integrated Units

	E-100	DT-201 Condenser
Q (kW)	27.8	-470.63
Tin (°C)	25	194
Tout (°C)	120	

The condenser stream can be used to replace the hot oil currently heating E-100. The heat duty of the heat exchanger remains the same since the condenser stream maintains the 10°C minimum temperature difference with the heater inlet. Additionally, the remaining heat duty needed for the reboiler can be calculated.

For the reboiler:

$$Q = -470.63 \text{ kW} + 27.81 \text{ kW} = -442.81 \text{ kW}$$

Additionally, the savings in heat duty can be used to calculate the total savings found for hot oil in the heat exchanger and chilled water in the condenser.

For hot oil savings:

$$Cost = 27.81 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{1 \text{ MMBTU}}{1,000,000 \text{ BTU}} \cdot \frac{2700 \text{ hr}}{\text{yr}} \cdot \frac{\$4}{\text{MMBTU}} = \$1,200/\text{yr}$$

For chilled water savings:

$$Cost = 27.81 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{\text{ton} - \text{day}}{288000 \text{ BTU}} \cdot \frac{4700 \text{ hr}}{\text{yr}} \cdot \frac{\$1.5}{\text{ton} - \text{day}} = \$2,300/\text{yr}$$

Lastly, the bare module capital costs for the heat exchangers can be calculated as following Appendix E, E-3.

Table D-2(II). Bare Module Costs after Heat Integration

	Installed Cost (Bare Module Cost)
E-100 (original HEX)	\$9,800
E-100A (new HEX replacing E-100)	\$8,600

The overall savings are summarized in the table below:

Table D-2(III). Savings due to Heat Integration

Capital Costs	<i>\$1,200</i>
Hot Oil Utilities	<i>\$1,200/yr</i>
Chilled Water Utilities	<i>\$2,300/yr</i>
Total Savings for Year 1	<i>\$4,800</i>
Total Utility Savings after Year 1	<i>\$3,500/yr</i>

D-3. Above the Pinch Sample Calculation

The two combinations of major energy requirements that were chosen for heat integration were: (1) the cooling in E-203 and the heating of the reboiler in DT-200 and (2) the cooling in E-204 and the heating of the reboiler in DT-201.

(1) E-203 and DT-200 Reboiler

The heat duty requirements and temperature values across the units were pulled from ASPEN.

Table D-3(I). Heat Integrated Units

	E-203	DT-200 Reboiler
Q (kW)	-14.36	90.72
T _{in} (°C)	214	200
T _{out} (°C)	25	

Using the temperature values from each unit, the new temperature differences in our network can be calculated, based on maintaining a minimum temperature difference of 10°C. The original heat exchanger, E-203, will be broken into two new heat exchangers, E-203A and E-203B. E-203A will be placed in the original location of E-203 and E-203B will be placed directly after the reboiler in DT-200. The heat duties of these two heat exchangers can be calculated from the temperature differences and must sum to equal the original heat duty of E-203. Additionally, the remaining heat duty needed for the reboiler can be calculated.

Table D-3(II). Heat Integration Temperatures

	E-203B	E-203A	DT-200 Reboiler
Q (kW)	-0.29	-14.07	90.43
T _{in} (°C)	214	210	200
T _{out} (°C)	210	25	

For E-203B:

$$Q = \frac{(214 - 210)^{\circ}\text{C}}{(214 - 25)^{\circ}\text{C}} * (-14.36\text{ kW}) = -0.29\text{ kW}$$

This heat duty from E-203B is equal to our savings. We can use this value to calculate the remaining heat duty left in the heat exchange E-203A and the heat duty still required for the reboiler in DT-200.

For E-203A:

$$Q = -14.36\text{ kW} - (-0.29\text{ kW}) = -14.07\text{ kW}$$

For the reboiler:

$$Q = 70.92\text{ kW} + (-0.29\text{ kW}) = 90.43\text{ kW}$$

Additionally, the savings in heat duty can be used to calculate the total savings found for chilled water in the heat exchanger and hot oil in the condenser.

For chilled water savings:

$$\text{Cost} = 0.29 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{\text{ton} - \text{day}}{288000 \text{ BTU}} \cdot \frac{2700 \text{ hr}}{\text{yr}} \cdot \frac{\$1.5}{\text{ton} - \text{day}} = \$24/\text{yr}$$

For hot oil savings:

$$\text{Cost} = 0.29 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{1 \text{ MMBTU}}{1,000,000 \text{ BTU}} \cdot \frac{4700 \text{ hr}}{\text{yr}} \cdot \frac{\$4}{\text{MMBTU}} = \$22/\text{yr}$$

Lastly, the bare module capital costs for the heat exchangers can be calculated as following Appendix E: E-5.

Table D-3(III). Bare Module Costs after Heat Integration

	Installed Cost (Bare Module Cost)
E-203 (original HEX)	\$9,200
E-203B (HEX placed after reboiler)	\$6,600
E-203A (new HEX replacing E-200)	\$9,200

The overall savings are summarized in the table below:

Table D-3(IV). Savings due to Heat Integration

Capital Costs	-\$6,600
Hot Oil Utilities	\$22/yr
Chilled Water Utilities	\$24/yr
Total Savings for Year 1	-\$6,500
Total Utility Savings after Year 1	\$46/yr

(2) E-204 and DT-201 Reboiler

The heat duty requirements and temperature values across the units were pulled from ASPEN.

Table D-3(V). Heat Integrated Units

	E-204	DT-201 Reboiler
Q (kW)	-1.45	467.64
T _{in} (°C)	287	216
T _{out} (°C)	25	

Using the temperature values from each unit, the new temperature differences in our network can be calculated, based on maintaining a minimum temperature difference of 10°C. The original heat exchanger, E-204, will be broken into two new heat exchangers, E-204A and E-204B. E-204A will be placed in the original location of E-204 and E-204B will be placed directly after the reboiler in DT-201. The heat duties of these two heat exchangers can be calculated from the temperature differences and must sum to equal the original heat duty of E-204. Additionally, the remaining heat duty needed for the reboiler can be calculated.

Table D-3(VI). Heat Integration Temperatures

	E-204B	E-204A	DT-201 Reboiler
Q (kW)	-0.34	-1.11	467.30
T _{in} (°C)	287	226	216
T _{out} (°C)	226	25	

For E-204B:

$$Q = \frac{(287 - 226)^{\circ}\text{C}}{(287 - 25)^{\circ}\text{C}} * (-1.45 \text{ kW}) = -0.34 \text{ kW}$$

This heat duty from E-204B is equal to our savings. We can use this value to calculate the remaining heat duty left in the heat exchange E-204A and the heat duty still required for the reboiler in DT-201.

For E-204A:

$$Q = -1.45 \text{ kW} - (-0.34 \text{ kW}) = -1.11 \text{ kW}$$

For the reboiler:

$$Q = 467.64 \text{ kW} + (-0.29 \text{ kW}) = 467.30 \text{ kW}$$

Additionally, the savings in heat duty can be used to calculate the total savings found for chilled water in the heat exchanger and hot oil in the condenser.

For chilled water savings:

$$\text{Cost} = 0.34 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{\text{ton} - \text{day}}{288000 \text{ BTU}} \cdot \frac{2700 \text{ hr}}{\text{yr}} \cdot \frac{\$1.5}{\text{ton} - \text{day}} = \$28/\text{yr}$$

For hot oil savings:

$$\text{Cost} = 0.34 \text{ kW} \cdot \frac{3214 \text{ BTU}}{\text{kWh}} \cdot \frac{1 \text{ MMBTU}}{1,000,000 \text{ BTU}} \cdot \frac{4700 \text{ hr}}{\text{yr}} \cdot \frac{\$4}{\text{MMBTU}} = \$26/\text{yr}$$

Lastly, the bare module capital costs for the heat exchangers can be calculated as following Appendix E, E-3.

Table D-3(VII). Bare Module Costs after Heat Integration

	Installed Cost (Bare Module Cost)
E-204 (original HEX)	\$6,200
E-204B (HEX placed after reboiler)	\$5,800
E-204A (new HEX replacing E-200)	\$6,100

The overall savings are summarized in the table below:

Table D-3(VIII). Savings due to Heat Integration

Capital Costs	-\$5,700
Hot Oil Utilities	\$26/yr
Chilled Water Utilities	\$28/yr
Total Savings for Year 1	-\$5,600
Total Utility Savings after Year 1	\$54/yr

APPENDIX E: UNIT SIZING AND CAPITAL COST SAMPLE CALCULATIONS

E-1. R-100

First, the amount of hot oil needed for running an isothermal reactor at 120°C was calculated. A heat duty value of -288 kW was used for the isothermal reactor, which was based on the heat of reaction per batch. Using Shell Thermia B, a temperature difference of 10°C was assumed. The amount of hot oil could be determined using the equation:

$$Q = mc\Delta T$$

$$m = \frac{Q}{c\Delta T} = \frac{576 \text{ kW/batch}}{(3.03 \text{ kJ/kg}^\circ\text{C}) \cdot 10^\circ\text{C}} = 5,557 \text{ kg/batch} = 2,778 \text{ kg/hr}$$

Next, the amount of surface area required to heat the reactor was calculated using the equation:

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

The value of ΔT_{LM} was calculated using the inlet and outlet temperatures of our cold and hot streams, the stream flowing through our reactor at 120°C, and the hot oil flowing in at 340°C and out at 330°C.

$$\Delta T_{LM} = \frac{(340 - 120) - (330 - 120)}{\ln\left(\frac{340 - 120}{330 - 120}\right)} = 215.12$$

The overall heat transfer coefficient was found in Table 12.5 in the textbook and was chosen based on a liquid-liquid media with naphtha on the shell side and oil on the tube side. This provided a range from 25 - 35 BTU/ft² hr °F (or 0.1420 - 0.1987 kJ/m² s K). The upper limit was chosen because the most efficient value for heat transfer was assumed to give the lowest surface area required. Using these values with the heat duty from ASPEN, the minimum required surface area could be calculated.

$$SA = \frac{Q}{U \cdot \Delta T_{LM}} = \frac{576 \text{ kW}}{(0.1987 \text{ kJ/m}^2 \text{ s K}) \cdot (215.12 \text{ K})} = 13.47 \text{ m}^2$$

The reactor volume was calculated based on catalyst loading and reactant volume.

Catalyst Loading:

$$V_c = \frac{m}{\rho} = \frac{18.88 \text{ kg}}{0.72 \text{ kg/L}} = 26.23 \text{ L} = 0.026 \text{ m}^3$$

Reactant Volume:

$$V_R = \frac{m}{\rho} = \frac{188.8 \text{ kg AA} + 1360.1 \text{ kg BA}}{\left[\left(1.05 \frac{\text{g}}{\text{cm}^3} \text{AA} \cdot 12\% \text{AA} \right) + \left(1.044 \frac{\text{g}}{\text{cm}^3} \text{BA} \cdot 88\% \text{BA} \right) \right] * 1000} = 1.48 \text{ m}^3$$

Total Material Volume:

$$V = V_C + V_R = 1.51 \text{ m}^3$$

By using the ratio between area and volume, dimensional analysis could be completed to solve for reactor diameter.

$$\begin{aligned} SA &= \pi \cdot D \cdot h \\ V &= \frac{\pi \cdot D^2 \cdot h}{4} \\ \frac{SA}{V} &= \frac{4 \cdot \pi \cdot D \cdot h}{\pi \cdot D^2 \cdot h} = \frac{4}{D} \\ D &= \frac{4 \cdot V}{A} = 0.45 \text{ m} \end{aligned}$$

By assuming a head space of 10% of the material volume, the height of the tank was found to be 10.5 m.

$$h = \frac{4 \cdot (1.1 \cdot V)}{\pi \cdot D^2} = 10.5 \text{ m}$$

The tall reactor is a direct result of the amount of heating required to maintain the reactor temperature. The isothermal batch reactor, R-100, includes an agitator and heating jacket. An autoclave was used to cost our reactor because they are both vertical, cylindrical stirred-tank reactor. The equation chosen for the autoclave costing used a material of stainless steel. These autoclaves are provided with turbine agitators and heat-transfer jackets.¹⁹

$$C_P = 2,245S^{0.58}$$

where S is a size factor for the vessel volume in gallons. For the batch reactor, the required volume is 390.72 gallons. To scale up the year, cost indices were used. Additionally, a factor of 1.4 was used for piping and circulation of the hot oil. Therefore, our purchase cost was calculated as:

$$C_P = 2,245(390.72^{0.58}) * \left(\frac{610}{567}\right) * 1.4 = \$107,739.07$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A factor of 4.16 was used for vertical pressure units. There, our bare module cost was calculated as:

$$C_{BM} = \$107,739.07 * 4.16 = \mathbf{\$448,195}$$

E-2. P-100

A pump (P-100) was required by R-100 to load and unload the liquids from the vessel. An external gear pump was used due to the smaller volumetric flowrate going through the pump. The purchase cost is given by:

$$C_P = F_M C_B$$

where F_M is a material factor and C_B is given by:¹⁹

$$C_B = \exp\{8.2816 - 0.2918[\ln Q] + 0.0743[(\ln Q)^2]\}$$

where Q is the volumetric flowrate applicable over a range of 10 to 900 gpm. Using the volumetric flowrate of 12.94 gpm,

$$C_B = \$3,045.94$$

A material factor of 2 was used for stainless steel. To scale up the year, cost indices were used. Therefore, our purchase cost was calculated as:

$$C_P = \$3,045.94 * 2 * \left(\frac{610}{567}\right) = \$6,553.87$$

An electric motor is required to run the pump, so the purchase cost was needed for the total purchase cost. The purchase cost for an electric motor is given as:

$$C_P = F_T C_B$$

where F_T is a motor-type factor applicable for electric motor power consumption (P_C) from 1 to 1,500 Hp and the base cost, C_B is given by:¹⁹

$$C_B = \exp\{5.9332 + 0.16829[\ln P_C] - 0.110056[(\ln P_C)^2] + 0.071413[(\ln P_C)^3] - 0.0063788[(\ln P_C)^4]\}$$

where P_C applies over the range of 1 to 700 Hp and is given by:¹⁹

$$P_C = \frac{QH\rho}{33,000\eta_P\eta_M}$$

where Q is volumetric flowrate in gpm, H is the pump head in feet, ρ is the liquid density in lb/gal and the efficiencies are given below.

Pump Fractional Efficiency:¹⁹

$$\eta_P = -0.316 + 0.24015(\ln Q) - 0.01199(\ln Q)^2$$

Motor Fractional Efficiency:¹⁹

$$\eta_M = 0.80 + 0.0319(\ln P_B) - 0.00182(\ln P_B)^2$$

Using $Q = 12.94$ gal/min and $P_B = 0.365$ hp, the efficiencies are calculated as:

$$\eta_P = 0.1139$$

$$\eta_M = 0.2916$$

Electric motor power consumption (P_C) was calculated as:

$$P_C = \frac{(12.94 \frac{gal}{min})(13.12 ft)(8.063 \frac{lb}{gal})}{(33,000)(0.1139)(0.2916)} = 1.25 hp$$

The base cost was then calculated as:

$$C_B = \$389.94$$

Using a motor-type factor of 1.7 for 1,800 rpm electric motors in an explosion-proof enclosure and scaling up the year using cost indices, the purchase cost was calculated as:

$$C_P = 1.7 * \$389.94 * \left(\frac{610}{567}\right) = \$713.18$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

The purchase costs of the pump and motor were added together. A bare module cost of 3.3 was used for pumps and drivers.

$$C_{BM} = (\$6,553.87 + \$713.18) * 3.3 = \mathbf{\$23,981}$$

E-3. R-101

A regeneration unit (R-101) was required to regenerate the catalyst for the reaction. The purchase cost is given by:

$$C_P = F_M C_V + C_{PL}$$

where F_M is a material factor, cost for an empty vertical vessel (C_V) is:¹⁹

$$C_V = \exp \{5.6336 + 0.4599[\ln(W)] + 0.00582[\ln(W)]^2\}$$

where W is the weight. Also, added costs of ladders and platforms (C_{PL}) for the vessel are calculated using inside diameter, D_i :¹⁹

$$C_{PL} = 2,275(D_i)^{0.2094}$$

The wall thickness (t_s) is 0.375 inches, inside vessel diameter (D_i) is 9.8452 inches, and ρ is 0.284 lb/in³. The weight is calculated as:¹⁹

$$W = \pi(D_i + t_s)(L + (0.8D_i))t_s\rho$$

where $L = 21.034$ m and $W = 98.826$ lb.

The cost for an empty vertical vessel is:

$$C_V = \$874$$

The added costs are as follows:

$$C_{PL} = \$783$$

For a material factor of 2.1 for stainless steel 316, the purchase cost was calculated as:

$$C_P = 2.1 * \$874 + \$783 = \$2,818$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A bare module factor of 3.05 was used for horizontal pressure vessels to calculate the bare module cost:

$$C_{BM} = \$2,818 * 3.05 = \$8,596$$

E-4. DT-200, DT-201, DT-202

The following sizing and installed cost calculation are the same for all three distillation towers. A summary of the important values has been provided at the end.

The tower diameter is given by:¹⁹

$$D_T = \left[\frac{4G}{(fU_f)\pi(1 - \frac{A_d}{A_T})\rho_G} \right]^{1/2}$$

where G is the vapor mass flow rate, f is a fraction, U_f is the vapor flooding velocity, A_d is the downcomer cross-sectional area, A_T is the tower cross-sectional area, and ρ_G is the vapor density. The value of f is typically 0.75 to 0.85, so a value of 0.80 was used.¹⁹ The value of $\frac{A_d}{A_T}$ is typically 0.10-0.20, so 15% was used.¹⁹

The vapor flooding velocity is given by:

$$U_f = C_{SB}F_{ST}F_F F_{HA} \left(\frac{\rho_L - \rho_G}{\rho_G} \right)^{1/2}$$

Once the tower diameter was found, the tower cross-section area could be calculated as:

$$A_T = \pi \cdot \left(\frac{D_T}{2} \right)^2$$

The packed height (H_P) of the column is given by:

$$H_P = HETP \cdot N_{equilibrium}$$

where $N_{equilibrium}$ is the number of stages in the column and HETP is given by:

$$HETP = 1.5 \cdot D_p$$

where D_p is the diameter of the packing. For all three distillation columns, ceramic Raschig rings of 0.5 in were used for packing since the tower diameters was less than 2.5ft. Therefore, the HETP was calculated to be 0.75.

The purchase cost of a packed tower is given by:

$$C_p = F_M C_V + C_{PL} + V_P C_{PK} + C_{DR}$$

where F_M is 2.1 for stainless steel 316 to prevent corrosion from acids, C_V is for an empty vertical tower, C_{PL} is for platforms and ladders, V_P is the packing volume, C_{PK} is the installed packing cost of \$20/ft³, and C_{DR} is the installed high-performance liquid distributor cost. It was assumed that one distributor was placed every 20 ft for the total column height with a cost of \$140/ft².

The vessel cost is given by:

$$C_V = \exp \{10.5449 - 0.4672[\ln(W)] + 0.05482[\ln(W)]^2\}$$

where W is the weight of the column and is calculated by:

$$W = \pi(D_i + t_s)(L + 0.8D_i)t_s\rho$$

where L is the height of the column, D_i is the inside tower diameter, t_s is the shell thickness = 0.375 in, and ρ is the density of carbon steel (490 lb/ft³)

The platform & ladder cost is given by:

$$C_{PL} = 341(D_i)^{0.63316}(L)^{0.80161}$$

To scale up the year, cost indices were used. Therefore, our purchase cost was calculated as:

$$C_P = (F_M C_V + C_{PL} + V_P C_{PK} + C_{DR}) * \left(\frac{610}{567}\right)$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A factor of 4.16 was used for vertical pressure units.

Table E-4(I). Sizing and Costing of the Distillation Columns

	DT-200	DT-201	DT-202
D_T (ft)	1.20	2.41	0.53
A_T (ft ²)	1.14	4.57	0.22
N_{eq}	12	94	10
H_p (ft)	9	70.5	7.5
H (ft)	13.5	84.5	9.5
C_V	\$4,844	\$54,229	\$1,525
C_{PL}	\$1,923	\$19,268	\$602
V_P	10.22	322.4	1.68
C_{DR}	\$159	\$4,481	\$31
C_P	\$13,400	\$155,000	\$4,200
C_{BM}	\$55,800	\$644,800	\$17,300

Additionally, the reboiler and condenser for each column was costed as a heat exchanger. See Appendix E-3 for the sample calculation. The purchase cost for each column, reboiler, and condenser are displayed below as well as the total for the entire column.

Table E-4(II). Total Bare Module Capital Costs

	DT-200	DT-201	DT-202
Column C_{BM}	\$55,800	\$644,800	\$17,300
Reboiler C_{BM}	\$21,400	\$21,700	\$23,700
Condenser C_{BM}	\$9,800	\$8,700	\$8,500
Total C_{BM}	\$87,000	\$675,200	\$49,500

E-5. Heat Exchangers (Heater + Cooler)

Heater

A Heat Exchanger (E-100) was required to heat the feed streams before entering the reactor. The purchase cost is given by:

$$C_P = F_M F_p F_L C_B$$

where F_M is a material factor, F_p is a pressure factor, F_L is a length factor, and C_B for a double-pipe heat exchanger is given by:

$$C_B = \exp\{8.2816 - 0.2918[\ln A] + 0.0743[(\ln A)^2]\}$$

where A is the area of the heat exchanger. The area of the heat exchanger was calculated using

$$Q = UA\Delta T_{lm}$$

where the heat transfer (Q) is determined from the ASPEN Plus simulation, and the overall heat transfer coefficients (U) were literature values assuming a liquid-liquid media and oil for the tube side. The temperature driving force (ΔT_{lm}) is given by:¹⁹

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln \left(\frac{\Delta T_2}{\Delta T_1} \right)}$$

Using the heat transfer of 27.81 kW, overall heat transfer coefficients of 0.14196 kJ/m²-s-K and 0.19874 kJ/m²-s-K, and temperature driving force between using the heat exchanger and hot oil of 155.38 K, the range of areas for the heat exchangers are:

$$A = 0.90069m^2 - 1.2610 m^2$$

Using the average area of 11.634 ft²,

$$C_B = \$2,131.20$$

Scaling up the year using cost indices, the base cost was calculated as:

$$C_B = \$2,131.20 * \frac{610}{567} = \$2,292.80$$

A material factor of 2 was used for stainless steel (inner) and carbon steel (outer), and the length factor is 1. The pressure factor is calculated as:¹⁹

$$F_p = 0.851 + \left(0.1292 * \frac{P}{600}\right) + \left(0.0198 * \frac{P}{600}\right) = 0.851$$

where P is zero.

The purchase cost was multiplied by a factor of 1.4 to account for piping and circulation system:

$$C_p = 1.4 * \$2,292.80 * 0.851 * 2 * 1 = \$5,463.27$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_p * F_{BM}$$

A bare module factor of 1.8 was used for double-pipe heat exchangers to calculate the bare module cost:

$$C_{BM} = \$5,463.27 * 1.8 = \$9,833.89$$

Coolers

A Heat Exchanger (E-203) was required to cool the benzyl acetate product before storage. The purchase cost is given by:

$$C_p = F_M F_p F_L C_B$$

where F_M is a material factor, F_p is a pressure factor, F_L is a length factor, and C_B for a double-pipe heat exchanger is given by:¹⁹

$$C_B = \exp\{8.2816 - 0.2918[\ln A] + 0.0743[(\ln A)^2]\}$$

where A is the area of the heat exchanger. The area of the heat exchanger was calculated using

$$Q = UA\Delta T_{lm}$$

where the heat transfer (Q) is determined from the ASPEN Plus simulation, and the overall heat transfer coefficients (U) were literature values assuming a liquid-liquid media and water for the tube side. The temperature driving force (ΔT_{lm}) is given by:¹⁹

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln \left(\frac{\Delta T_2}{\Delta T_1} \right)}$$

Using the heat transfer of -14.36 kW, overall heat transfer coefficients of 0.283915 kJ/m²-s-K and 0.851745 kJ/m²-s-K, and temperature driving force between using the heat exchanger and hot oil of 70.521 K, the range of areas for the heat exchangers are

$$A = 0.23912m^2 - 0.71737m^2$$

Using the average area of 5.1478 ft²,

$$C_B = \$1,870.52$$

Scaling up the year using cost indices, the base cost was calculated as:

$$C_B = \$1,870.52 * \frac{610}{567} = \$2,012.38$$

A material factor of 3 was used for stainless steel, and the length factor is 1. The pressure factor is calculated as:

$$F_p = 0.851 + \left(0.1292 * \frac{P}{600} \right) + \left(0.0198 * \frac{P}{600} \right) = 0.851$$

where P is zero.

The purchase cost was calculated as:

$$C_P = \$2,292.80 * 0.851 * 3 * 1 = \$5,137.59$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A bare module factor of 1.8 was used for double-pipe heat exchangers to calculate the bare module cost:

$$C_{BM} = \$5,137.59 * 1.8 = \mathbf{\$9,247.67}$$

E-6. Storage Tanks

Storage tanks were used for raw materials, intermediate tanks, and finished products.

Raw Materials

A storage tank (ST-101) was used to store benzyl alcohol before sent to the reactor. The purchase cost is given by:

$$C_P = n_{totes} C_{totes}$$

where the number of totes is calculated by the volume of benzyl alcohol required every two weeks divided by the volume of one tote, and two sets of totes are needed:

$$n_{totes} = 2 \text{ sets} * \frac{V_{BA}}{V_{tote}}$$

The volume of benzyl alcohol needed every two weeks is calculated by the mass (m) and density of benzyl alcohol (ρ)

$$V_{BA} = 2 \text{ weeks} * \frac{m}{\rho} = 3,237.06 \text{ gal}$$

The number of totes is calculated to be 24 totes. The purchase cost is calculated as:

$$C_P = \$6,480.00$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost to account for shipping, tax, and delivery.

$$C_{BM} = C_P * F_{BM}$$

A bare module factor of 1.5 was used for the totes to calculate the bare module cost:

$$C_{BM} = \$6,480.00 * 1.5 = \mathbf{\$9,720.00}$$

At the end of two weeks, water is sent in totes for wastewater treatment and dibenzyl ether is sold by the tote. The capital costs for these totes are calculated the same as raw material totes.

Intermediate Tanks

A stainless-steel floating roof storage tank (ST-103) was used to store mainly benzyl alcohol with acetic acid before recycled to the reactor as feed for the reaction. Scaling up to this year using cost indices, the purchase cost is given by:¹⁹

$$C_P = 2 * 475 V_{\text{tank}}^{0.507} \left(\frac{V_{\text{reactants}}}{V_{\text{tank}}} \right) \left(\frac{610}{567} \right)$$

Using a volume of reactants of 2,600 gallons and volume of tank of 30,000 gallons, the purchase cost is:

$$C_P = \$16,490.09$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A bare module factor of 3.05 was used for a horizontal pressurized vessel to calculate the bare module cost:

$$C_{BM} = \$16,490.09 * 3.05 = \mathbf{\$50,294.77}$$

Finished Products

A stainless-steel floating roof storage tank (ST-202) was used to store the finished product of benzyl acetate before being used in a subsequent process. Scaling up to this year using cost indices, the purchase cost is given by:¹⁹

$$C_P = 2 * 475 V_{\text{tank}}^{0.507} \left(\frac{V_{\text{reactants}}}{V_{\text{tank}}} \right) \left(\frac{610}{567} \right)$$

Using a volume of reactants of 4,021 gallons and volume of tank of 30,000 gallons, the purchase cost is

$$C_P = \$25,500$$

To find the bare module cost, a bare module factor is multiplied to the purchase cost.

$$C_{BM} = C_P * F_{BM}$$

A bare module factor of 3.05 was used for a horizontal pressurized vessel to calculate the bare module cost:

$$C_{BM} = \$25,500 * 3.05 = \textbf{\$77,777}$$

APPENDIX F. DISTILLATION START-UP SAMPLE CALCULATIONS

The following calculation is the same for all three distillation towers. A summary of the important values has been provided at the end.

The volume (L) to fill up each tray in the distillation tower is given by:

$$V_f = A_T \cdot h_w \cdot N_{actual}$$

where A_T is the tower cross-sectional area in m^2 , h_w is the weir height = 0.0508m, and N_{actual} is the actual number of stages in the column. The actual number of stages can be found using:¹⁹

$$N_{actual} = \frac{N_{equilibrium}}{E_o}$$

where the overall tray efficiency (E_o) was calculated using the O'Connell Correlation:¹⁹

$$E_o = 50.3(\alpha\mu)^{-0.226}$$

where α is the average volatility and μ is the viscosity of the feed in cP.

The time to fill up the distillation column is given by:

$$t_f = \frac{V_f}{B}$$

where B is the total boil-up rate in (L/hr). The total boil-up rate was calculated by adding the flowrates of the vapor going back into the column from the reboiler and the bottoms leaving the reboiler.

The time for start-up is given by:

$$t_{su} = 5 \cdot t_f$$

Table F(I). *Distillation Column Values*

	DT-200	DT-201	DT-202
D_T (ft)	1.20	2.41	0.53
A_T (ft ²)	1.14	4.57	0.22
N_{eq}	12	94	10
α	1.85	2.07	5.87
μ (cP)	0.276	0.195	0.318
E_o	59%	62%	44%
N_{actual}	20	152	23
V_f (L)	109.8	3283.7	24.2
B (L/hr)	1245.79	5000.2	206.9
t_f (hr)	0.088	0.67	0.117
t_{su} (hr)	0.44	3.28	0.59

APPENDIX G. ADDITIONAL CAPITAL COSTS

G-1. Steam Generation and Oil Recirculation

Steam generation and oil recirculation are used to transfer heat in the process. The total purchase cost is calculated as:

$$C_P = C_{steam\ boiler} + C_{piping+circulation} + C_{hot\ oil}$$

where the cost of the steam boiler is:

$$C_{steam\ boiler} = 0.416 \left(\frac{Q}{0.85} \right)^{0.77}$$

and the cost of the hot oil is:

$$C_{hot\ oil} = 13.97Q^{0.64}$$

Using a total heat per year (Q) of 2.12×10^6 BTU/year, the cost of the steam boiler is:

$$C_{steam\ boiler} = \$35,052.53$$

and the cost of the hot oil is:

$$C_{hot\ oil} = \$156,333.25$$

The cost of the piping and circulation system is calculated as:

$$C_{piping+circulation} = 0.4C_{steam\ boiler} = \$14,021.01$$

Scaling up to this year using cost indices, the total purchase cost is:

$$C_P = (\$35,052.53 + \$14,021.01 + \$156,333.25) * \left(\frac{610}{567} \right) = \$220,984.38$$