

Plant Design and Profitability Analysis for the Production of Ethyl Acetate from Renewable Ethanol Feedstock

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Executive Summary

This is a techno-economic assessment of a 50 kta ethyl acetate production conceptual design. This is potentially a profitable venture that uses renewable ethanol feedstock reacting over a metal catalyst in an 8 m³ isothermal packed bed reactor at 240 °C and 2 atm. This design requires 24 MJ of energy per MT of ethyl acetate produced. The CO₂ produced by this process is of interest because of the sustainable motivations behind this project. This proposed design produces 0.19 kg of CO₂ per kg of ethyl acetate. This plant is proposed to last 15 years, over which time it will produce ethyl acetate worth \$1,100 per metric ton from ethanol worth \$500 per metric ton. This price difference yields a Net Present Value (NPV_{project}) of \$51 MM and a before tax Return on Investment (ROI_{BT}) of 41% through the annual before tax profit of \$14 MM. Additionally, the plant's IRR of 23% is well above the corporate enterprise rate of 10%, offsetting the risk of the Total Capital Investment of \$35 MM. The percent annual growth relative to this TCI, the NPV%, is 9% which normalizes for the investment and the plant lifetime. Based on this level of profitability, it is recommended that project research be continued to obtain better cost estimates and confirm the value of this potential investment.

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1. Introduction

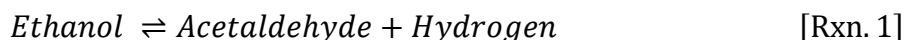
We propose a 50 kta conceptual design that produces ethyl acetate from ethanol feedstock derived from corn fermentation. The current global annual demand for ethyl acetate is 5 million metric tons with projected growth of 4.5% through 2025.^{1,2} Green Solvents Inc. is investing in renewable ethyl acetate production, suggesting a market demand for non-petroleum derived ethyl acetate. Specifically, in the production of renewable oxygenated solvents, which are used in paints, inks, pharmaceuticals, and cosmetics. This design attempts to capture an all new market for ethyl acetate, and as a renewable source, can provide an opportunity to positively impact the market. As consumers become more environmentally conscientious and carbon footprints are more important to the market, reducing CO₂ emissions improves a corporation's image such that it is not only the right ethical decision, it is the right economic decision as well.

Table 1. Economic Data

Substance	Price
Ethanol	\$500/MT
Ethyl Acetate	\$1,100/MT
Diethyl Ether	fuel value only
Hydrogen	fuel value only
Fuel	\$2.50/MM BTU
Catalyst	\$10,000/MT
CO ₂ Charge	\$40/MT

1.1 Reaction Chemistry

Ethyl acetate will be produced via a two-step catalytic reaction on the surface of the a 94:5:1 mass ratio catalyst of CuO, CoO, and Cr₂O₃, respectively.



The second reaction occurs very rapidly, however, and these two reactions can be simplified to:



In addition, the following side reaction which dehydrates ethanol to diethyl ether and water takes place at one tenth the speed of the main reaction.



This reaction set is approximated with Langmuir-Hinshelwood kinetics. The lab-scale experiments performed have been scaled based on the surface area of the larger catalyst particles in the reactor, resulting in the following kinetics which account for the mass transfer to and into the catalyst.

$$r_{EA} \left[\frac{\text{mol}}{\text{hr g} \cdot \text{cat}} \right] = \frac{kK_E \left[p_E^2 - \frac{p_{EA}p_{H_2}^2}{K} \right]}{\left[1 + K_E p_E + K_{EA} p_{EA} + K_{H_2} p_{H_2} \right]^2} \quad [1]$$

$$K \text{ [atm]} = \exp \left(\frac{-3127}{T} + 5.32 \right) \quad [2]$$

$$k \left[\frac{\text{mol}}{\text{hr g} \cdot \text{cat atm}} \right] = \exp \left(\frac{-16310}{RT} + 10.95 \right) \quad [2]$$

$$K_E \text{ [atm}^{-1}] = \exp \left(\frac{5890}{RT} - 6.40 \right) \quad [2]$$

$$K_{EA} \text{ [atm}^{-1}] = \exp \left(\frac{11070}{RT} - 9.40 \right) \quad [2]$$

$$K_{H_2} \text{ [atm}^{-1}] = \exp \left(\frac{6850}{RT} - 7.18 \right) \quad [2]$$

Because the secondary reaction constantly consumes ethanol at 10% the rate of the main reaction, the selectivity towards the desired ethyl acetate is constant. The isothermal reactor design is also dependent on the heat of reaction, listed below.

$$\Delta H_{Rxn,1} = 26 \frac{\text{kJ}}{\text{mol product}} \quad [5]$$

2. Plant Design

2.1 Conceptual Design Overview

The dehydration of ethanol is carried out in an isothermal packed bed reactor (PBR). The reaction has a positive (endothermic) heat of reaction that is counteracted by a heated reactor design in order to maintain an appropriate reactor temperature throughout the length of the tubes. A packed bed reactor has been chosen such that the heterogeneous reaction can be performed without concern for inhomogeneous catalyst mixing which would be required to simulate a CSTR. Furthermore, neither large heat transfer nor continuous catalyst regeneration are needed, so a fluidized bed reactor (FBR) is unnecessary. The catalyst, a mixture of copper oxide, cobalt oxide, and chromium (III) oxide, used in this reaction is expected to be replaced twice annually at our desired production rate of 50 kta.

The maximum economic potential for this reaction mechanism is approximately \$29 MM annually, which equates to \$550 per kg of ethanol feedstock. These calculations are based on the values of ethyl acetate and ethanol remaining constant at \$1,100 and \$500 per MT, respectively. This was large enough to proceed with a Level 2 analysis of the process design. At Level 2 where only ethanol is fed to the plant, ethanol is completely recycled within the plant while ethyl acetate, diethyl ether, water, and hydrogen gas exit the plant. Since the second reaction happens at one tenth the speed of the first reaction, the selectivity is constant value at 0.45 and is independent of conversion. Selectivity is defined as the molar flow of ethyl acetate product divided by the molar

flow of fresh ethanol feed. Diethyl ether and hydrogen have value only as a fuel source and water must be disposed of.

Proceeding with the unit operations and recycle structure, it was found to be beneficial to combust the hydrogen and diethyl ether to produce steam throughout the plant. To recover energy from our reactor effluent prior to separation, it is used to heat the reactor feed to saturation temperature. After leaving this exchanger, the reactor effluent is further cooled with chilled brine to approximately 0°C before entering the separation system. This is necessary because in the hydrogen flash unit, more ethyl acetate will be lost as a vapor if the stream is at a higher temperature. After being heated by the reactor effluent, the reactor feed is vaporized and superheated in a steam kettle reboiler and a steam heat exchanger, respectively.

The separation system for this design needs to perform a liquid separation of all components leaving the reactor. With exit points for all components, a purge stream is unnecessary. The separation system for this design starts with a flash separation of hydrogen from the remaining four components. The flash is performed at 2 atm and 0°C in order to maximize recovery of ethyl acetate in the liquid stream. Diethyl ether is assumed to have perfect separation (using a split block), but further analysis should be done to get a more realistic process design. This design might include a liquid extraction system. Next, a separation of ethyl acetate, water, and ethanol is performed. Due to the azeotropes present in this ternary mixture, a pressure swing distillation sequence is used in a series of 2 columns. The first column has a bottoms stream of nearly pure ethanol (with a small amount of water) and a distillate stream of an ethyl acetate enriched ternary mixture. This first column operates at atmospheric pressure as this preliminary enrichment does not need to cross any azeotropes. The second column takes the ternary mixture and produces ethyl acetate in the bottoms and a mixture of water and ethanol in the distillate. This second column must operate at 20 atm to perform this separation successfully. The azeotrope between ethyl acetate and ethanol exists for all pressures below approximately 18 atm when using the NRTL model (Appendix D). The water-ethanol mixtures from the bottoms of column one and distillate of column two are then mixed and separated using pressure swing adsorption (PSA). The ethanol-water azeotrope can be broken using a spherical 3A zeolite to adsorb water. This allows the ethanol stream to have up to 99.6% purity, exceeding the azeotropic purity of 95%.³

2.2 Conceptual Design Variable Discussion

Reactor temperature, pressure, and per pass conversion are the variables that have been adjusted and used to optimize the design. The production rate of ethyl acetate is fixed at 50 kta. Simulations were performed for a range of per pass ethanol conversion and a range of temperatures and pressures from 225°C to 240°C and 2 atm to 10 atm, respectively. At constant pressure, the reactor volume decreases as temperature increases. Higher temperatures increase the rate of forward reaction for reactions 1 and 2, which means a smaller reactor volume is required to achieve the same extent of reaction. At constant temperature and low conversion, reactor volume decreases as pressure increases. However, for each pressure there exists a critical conversion where the reactor volume begins to increase exponentially as the reactions approach equilibrium (Appendix A.1.2). At low conversion, the mole fraction (equivalently partial pressure) of ethyl acetate and hydrogen is sufficiently small such that the forward reaction rate increases as pressure increases. The critical conversion is present because reaction 1 generates and consumes moles in a 3:2 ratio and the rate of reaction is dependent on the partial pressures of ethanol, ethyl acetate, and hydrogen.

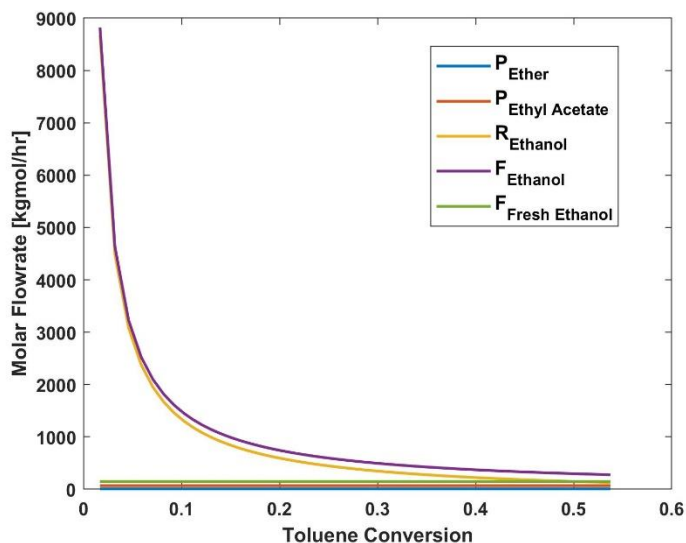


Figure 2. Molar Flow Rates of recycle and ethanol feed decrease while molar flow rates of product streams remain constant as reactor conversion increases.

To minimize the reactor volume the operating temperature and pressure have been selected to be 240°C and 2 atm. Operating at the lower limit of per pass ethanol conversion is impractical due to the exponential increase in flow rates to the reactor and through the separation system. Further, the process has an upper bound on conversion of approximately 55% due to equilibrium limitations. To optimize the conversion, a separation system was designed for 5 different conversions between 30% and 50%. After costing the 5 different process conditions we found that 45% conversion was the most cost effective choice and is used for all further modeling.

2.3 Aspen HYSYS Simulation

The reactor was modeled as an isothermal plug flow reactor at 2 atm and 240 °C. A heating input of 0.6 MW is required for isothermal reactor operation. Pressure drop across the reactor was assumed to be 0.5 atm. Accounting for non-ideal fluid properties and reactor pressure drop, the reactor volume was determined to be 8 m³ with a void fraction of 0.5. This corresponds to a per pass ethanol conversion of 45.1%. A flash drum creates a vapor stream of 97% hydrogen. The liquid stream off the flash drum contains 0.02% hydrogen. A separator block is used to remove the remaining hydrogen and all diethyl ether. The first distillation column operates at 1 atm and enriches ethyl acetate in the distillate. The feed stream to the first column is 70% ethanol, 27% ethyl acetate, and 3% water. The enriched distillate is 44% ethanol, 52% ethyl acetate, and 4% water. The distillate is fed to the second column at 20 atm and produces a pure stream of ethyl acetate. Distillation columns were modeled in Aspen Plus V10 using UNIQUAC to model vapor liquid properties. The streams not enriched with ethyl acetate are combined and fed to a split block. The split block simulates a pressure swing adsorption system. Leaving the PSA unit the recycled stream is primarily ethanol with some ethyl acetate that was not separated by the second column. Other distillation schemes were investigated in Aspen Plus and determined to be infeasible due to the extreme stage numbers and reflux ratios required. Despite our confidence in the accuracy of the kinetics, especially in the HYSYS simulation, the 8m³ reactor is unreasonably small and realistically, it is expected that a reactor would be closer to 10 times this value. For the purposes of the design economics, the 8 m³ reactor has been used, but comparisons to a larger reactor have been made such that the effect of inaccurate kinetics can be determined.

2.4 Process Flow Diagram

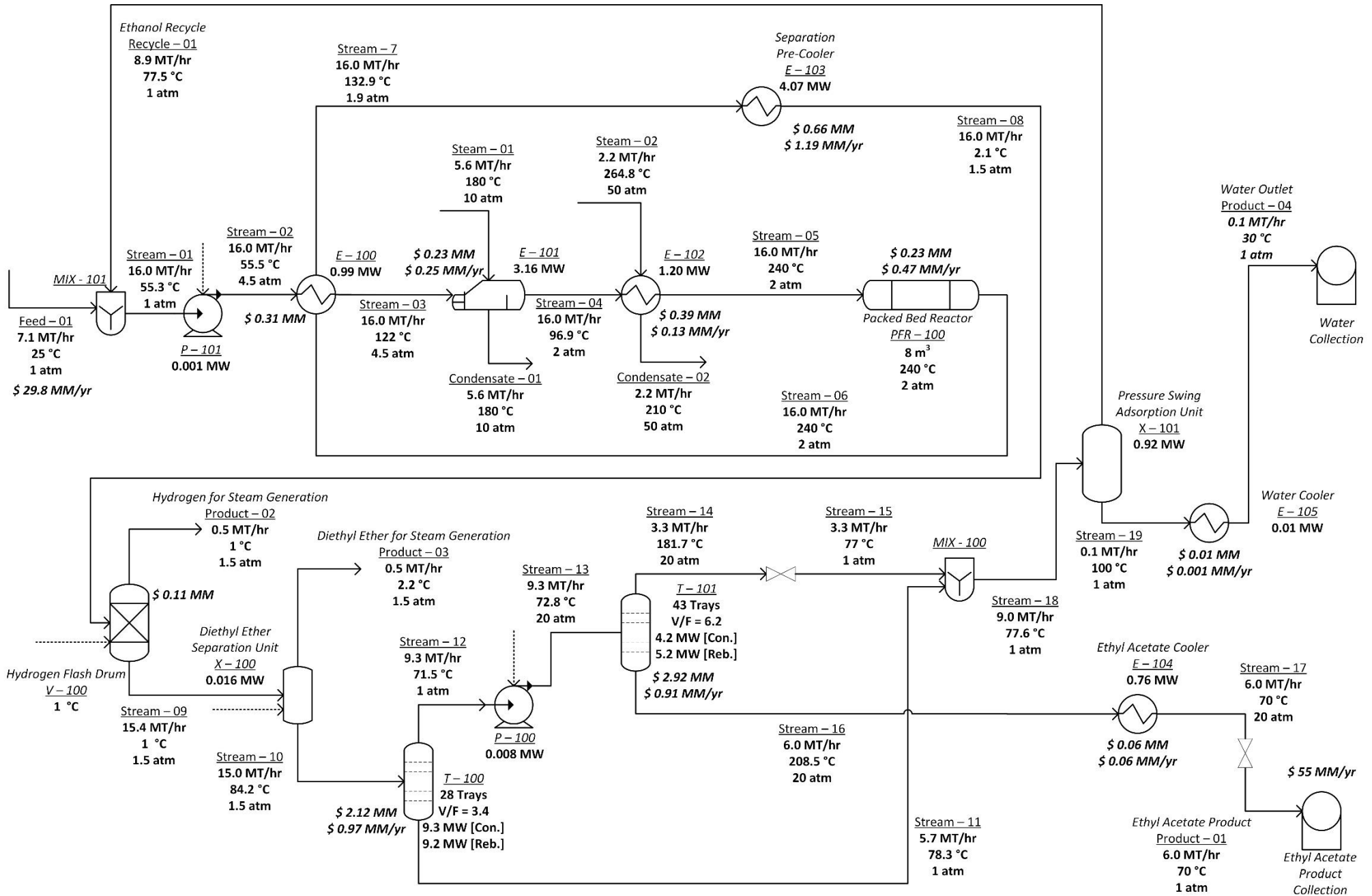


Figure 3. Detailed process flow sheet with stream conditions and mass flow rates.

2.5 HYSYS Flowsheet

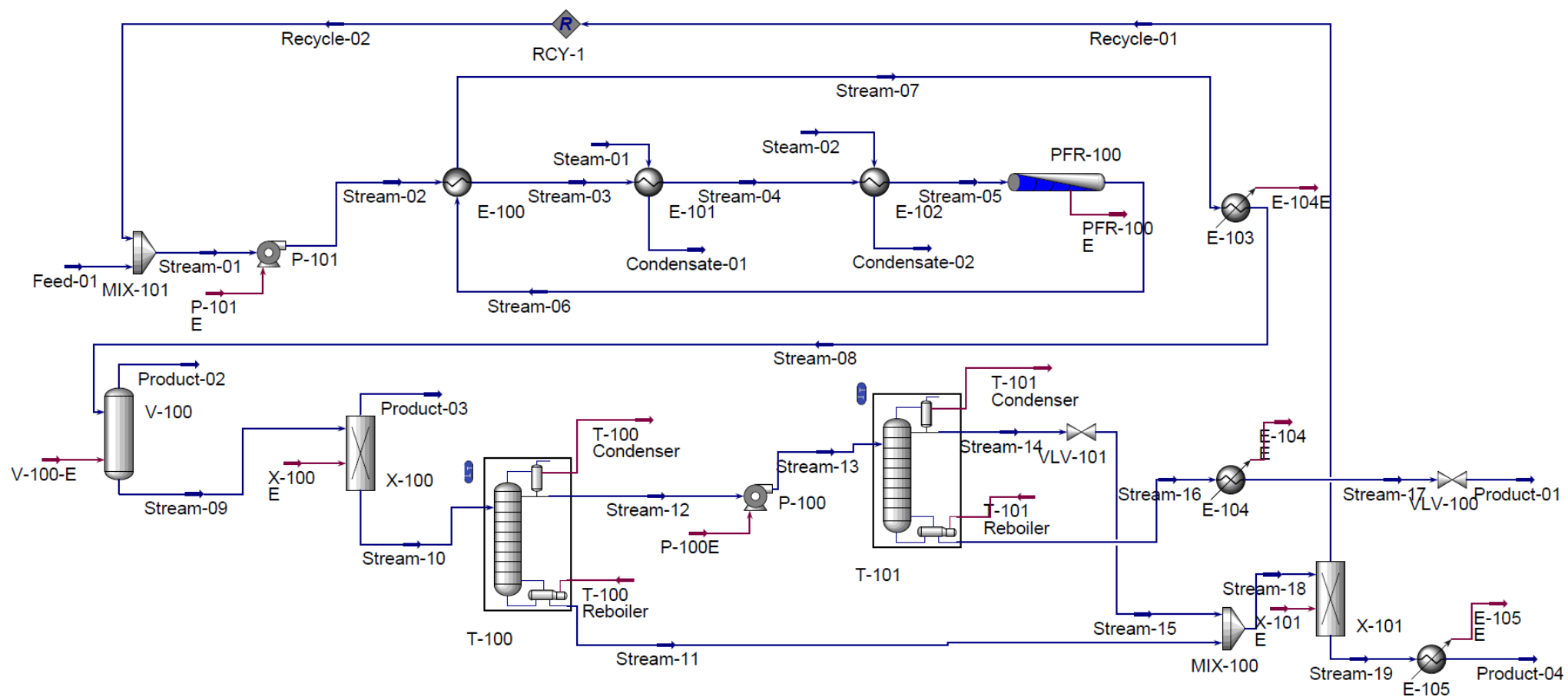


Figure 4. HYSYS simulation flow sheet. Stream conditions, energy, and mass flow rates can be found in Appendix E.

3. Economic Analysis

This design is possibly a good investment. The annual projected profit before taxes (P_{BT}) at the desired production rate is \$14 MM with a Total Capital Investment (TCI) of \$35 MM. TCI accounts for capital required to purchase and install plant equipment as well as administrative buildings, startup costs, and other plant facility costs. In addition, a 100% contingency is included to account for possible costs associated with additional equipment required. A breakdown of the plant equipment and annual operating costs are shown in Table 2. The primary metric used to determine and optimize plant profitability is the normalized Net Present Value of the project, $NPV\%$, which is calculated by discounting the cash flows from each year of plant construction and operating life back to the Board's decision time. When simulated in HYSYS and fully costed, the base-case of 45% conversion yields an NPV_{project} of \$51 MM and $NPV\%$ of 9%.

Table 2. Estimated project capital and operating costs

Equipment	Installed Cost [\$MM]	Operating Cost [\$MM/y]	Size	Duty [MW]
PFR-100	0.22	0.05	8 m ³	0.6
Heat Exchanger E-100	0.31	-	103 m ²	-
Heat Exchanger E-101	0.23	0.25	55 m ²	3.2
Heat Exchanger E-102	0.39	0.13	188 m ²	1.2
Heat Exchanger E-103	0.66	1.2	131 m ²	4.1
Heat Exchanger E-104	0.06	0.06	11 m ²	0.6
Heat Exchanger E-105	0.006	0.0008	0.3 m ²	0.01
Distillation Column T-100	1.2	-	17 m, 28 trays	-
T-100 Reboiler	0.48	0.57	260 m ²	9.2
T-100 Condenser	0.44	0.67	335 m ²	9.3
Distillation Column T-101	2.0	-	26 m, 43 trays	-
T-101 Reboiler	0.50	0.60	498 m ²	5.2
T-101 Condenser	0.47	0.30	466 m ²	4.2
Flash Drum V-100	0.11	-	3.3 m ³	-
Adsorption Column X-100	0.10	0.02	-	0.9
PSA X-101	0.16	0.07	-	0.4
Raw Ethanol	-	29.8	-	-
Administration & General Services	-	5.5	-	-
Catalyst Cost	-	0.50	-	-
CO2 Cost	-	0.37	-	-
Total Equipment Costs	7.3	-	-	-
Fixed Capital Investment	27	-	-	-
Total Investment	35	-	-	-
Working Capital	-	5.0	-	-
Revenue	-	55	-	-
Total Operating Costs	-	41	-	-

Due to the complexities of the separation system described earlier, the design could only be costed at discrete points, which were then compared to optimize the NPV%. Figure 6 shows the relationship between the NPV_{project} as well as the NPV% and the conversion of the reactor at 2 atm and 240 °C. From this plot, a conversion of 45% has been chosen as the operating point. Temperature and pressure were also varied and their effects on the design's economics were evaluated. Increasing the temperature to the practical maximum of 240 °C is most desirable as it decreases the volume of the reactor for a given conversion. The relationship between NPV_{project} and temperature for various conversions while ignoring the separations system can be seen in Appendix A.2.1., and from this relationship it is clear that the higher temperature reactor is more cost effective as the reactor size shrinks. At low conversions, a higher pressure yields a marginally smaller reactor and therefore less expensive TCI for the design, however, lowering the pressure increases the equilibrium conversion of the reactions and consequently allows the separations system to operate in a more feasible regime (Appendix A.2.2). NPV% was optimized rather than NPV_{project} because the difference in NPV_{project} between 40% conversion and 45% conversion was only approximately \$1 MM, while the higher conversion decreases the total capital investment of the design by over \$4 MM. The marginal increase in project value was determined to be worth less than the decrease in upfront costs. If the Board wishes to only maximize the NPV_{project}, then a conversion of 40% is recommended instead.

As mentioned previously, the kinetics provided yield a reactor volume of 8 m³ for a 45% conversion reactor. Based on this unreasonably small size, a larger reactor volume of 50 m³ has been substituted for the purposes of testing whether the NPV_{project} is sensitive to this potential error. With a 50 m³ reactor, the NPV_{project} drops to \$34 MM and the P_{BT} decreases to \$12 MM due to the expensive catalyst cost. This large change in the expected profitability of the design highlights the importance of ensuring that the kinetics have been measured properly.

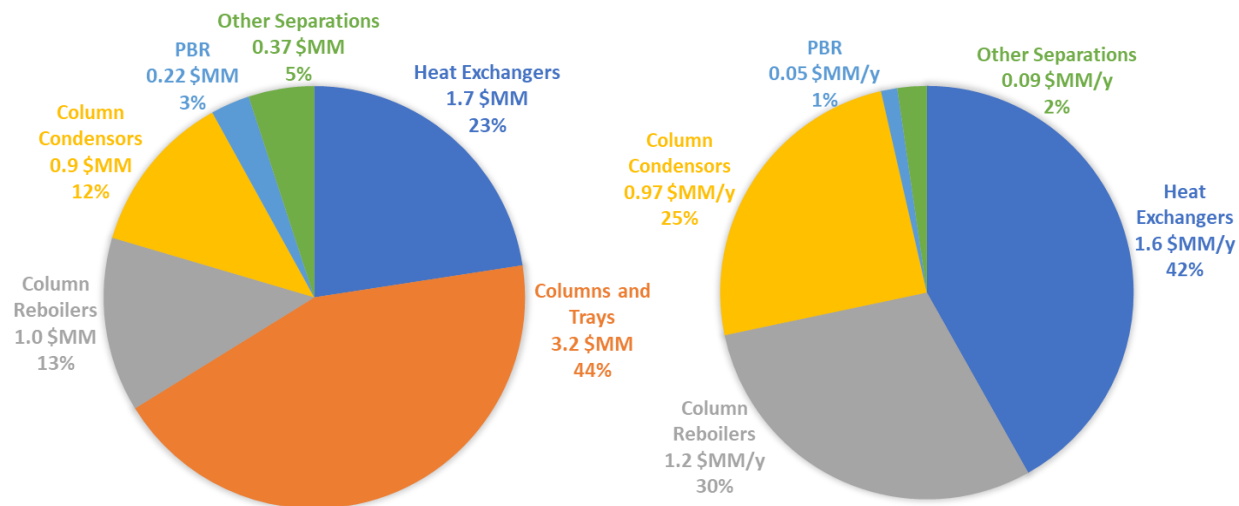


Figure 5. Comparison of equipment capital cost (left) and annual operating cost (right) for the selected design

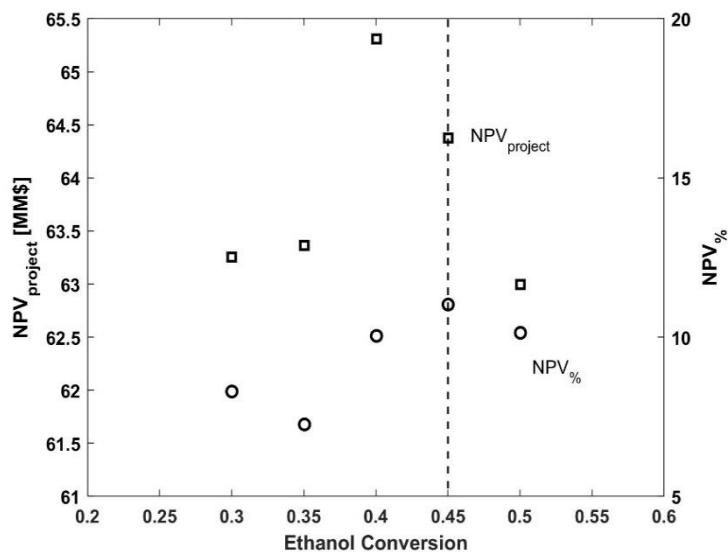


Figure 6. $NPV_{project}$ and $NPV\%$ vs conversion, calculated from the conceptual design and plotted based on Aspen Plus separations designs. Maximum $NPV\%$ occurs at a reactor conversion of 45%.

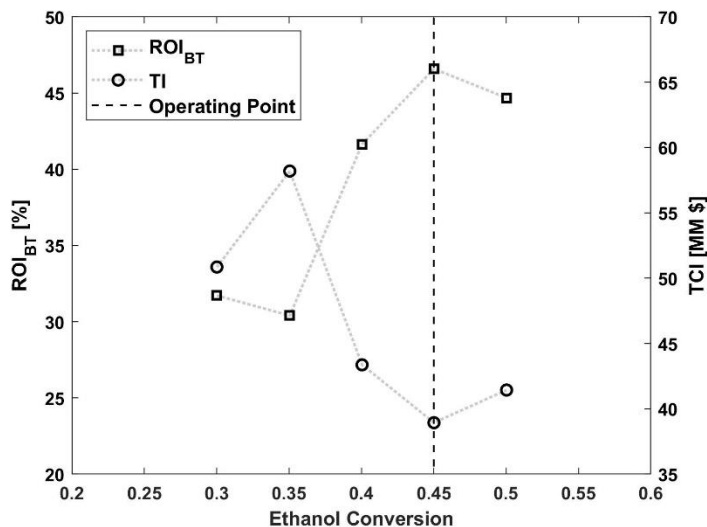


Figure 7. ROI_{BT} and TCI as functions of reactor conversion. The decrease in TCI shifts the maximum of the non-discounted ROI_{BT} towards higher conversions relative to NPV .

project to an unprofitable level. This is over ten times the highest carbon tax of any country.⁵ Because the reaction produces hydrogen which can be burned to create steam for the main unit operations of the plant, natural gas requirements are decreased and the carbon output of the design is low relative to its size.

In addition to the Net Present Value of the plant, the Return on Investment before taxes (ROI_{BT}) as well as the Internal Rate of Return (IRR) are useful metrics. The base-case yields an ROI_{BT} of 41% and an IRR of 23%. At a corporate enterprise earnings rate of 10%, this plant is profitable. These two metrics weigh the initial investment higher than $NPV_{project}$, shifting the optimum to a higher conversion, just as $NPV\%$ does. If the Board wishes to devote fewer resources to this project as we recommend, then these metrics assist in picking operating conditions at the cost of slightly less overall worth of the project.

One important factor in the design of this plant is the CO_2 production rate. To match the goals and motivations of the overall renewable ethyl acetate production, this plant should also aim to reduce its CO_2 footprint as much as possible. This is incorporated into the economic analysis as a \$40 per metric ton charge on CO_2 , paid towards CO_2 mitigation and capture projects. This also accounts for the possibility that in the next 15 to 20 years a CO_2 tax may be implemented. If this charge were not applied to the operation of the plant, the $NPV_{project}$ would increase by \$1.5 MM. The CO_2 charge would need to be raised to \$1465 per metric ton in order to reduce the

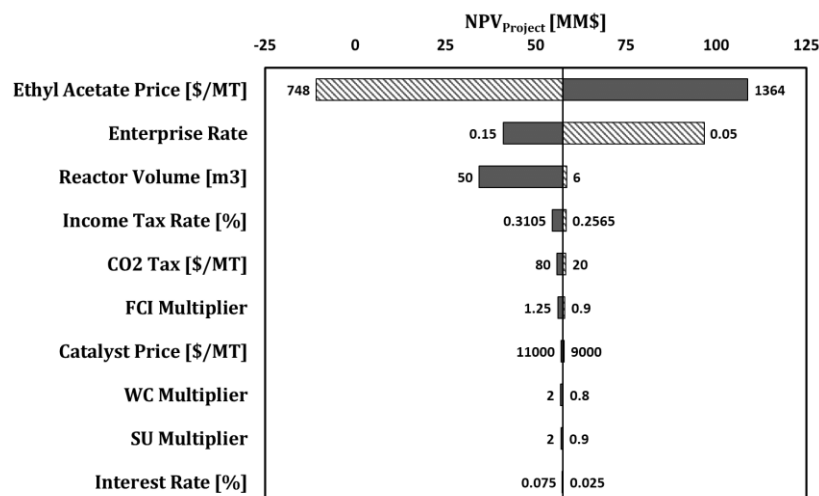


Figure 8. Sensitivity Analysis of $NPV_{project}$ based on typical bounds of parameter variation. Chemical price has largest effect of any design parameter or cost.

price as well as the enterprise rate at which cash flows are discounted. The reactor volume, which is in doubt, also can be seen in Figure 8, as the 50 m³ reactor would decrease the $NPV_{project}$ to \$34 MM. Changes in the fixed capital investment, working capital, and startup capital were also tested, yielding negligible changes to the project's net present value.

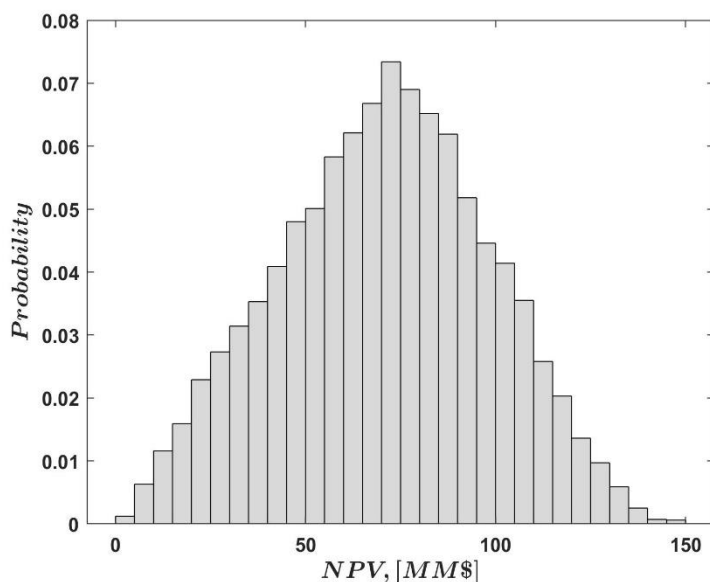


Figure 9. Probability density function of $NPV_{project}$ for Monte Carlo simulation with 10,000 randomized trials of economic parameters.

that there are market variations that last the entire 15 year lifetime of the plant, the project would remain profitable even if the price of ethyl acetate decreased by 17% to \$913 per MT, or the P_{BT} , which is analogous to the spread between the price of the products and the cost of manufacturing,

In addition to the economic analysis of the expected values for each price and rate, a sensitivity analysis was also performed to determine the expected change in the value of the ethyl acetate plant with respect to changes in the prices and rates^{6,7} (Appendix B). Ethyl acetate prices have been found to vary from as low as \$748 per metric ton to \$1364 per metric ton. These variations, along with those for other design variable variations, are displayed in Figure 8, show the strong dependence of plant profitability on the ethyl acetate

Stochastic simulations were used to generate a cumulative probability distribution for the $NPV_{project}$ given variations in the same set of prices and rates. Figure 9 shows the probability distribution of these Monte Carlo tests. The variables were assigned triangle distributions based on typical ranges in their values.⁶ Based on these simulations, there is a very small probability that the design will not be profitable given normal market fluctuations and production delays.

Based on the importance of chemical prices, theoretical market shocks of these prices were examined to find what scenarios the plant could withstand. If we assume

decreased by 61% to \$5.6 MM/y. If the plant were shut down immediately after startup for 6 years or less, perhaps due to a sudden recession or market change, it could still make enough profit to repay the bond principle in year 10.

In addition to market shocks, delays and unforeseen expenses during the construction phase can harm the profitability of the investment. These scenarios were simulated, and we found that if the construction process were delayed by one year, the NPV of the project would decrease by \$5 MM to \$46 MM. Similarly, if construction costs increased by 550%, corresponding to an increase in TCI to \$97 MM the plant would remain profitable, with an NPV of \$32 MM, while generating enough cash to repay the bond principle in year 10.

It should be noted that although the goal of this project is to use entirely bio-renewable ethanol, nothing about the equipment or design would need to be altered to process other ethanol of comparable purity if economic circumstances required it. These simulations and the flexibility of the feedstock shows a strong resilience to shifting markets and indicates the safety of this investment with respect to the variability in the chemical industry.

4. Materials of Construction

Carbon steels are compatible with all components for this process except the acetaldehyde intermediate. Thus, the reactor should be constructed using stainless steel as it is the lowest cost compatible material. Hydrogen embrittlement and slight ethanol corrosion can weaken carbon steel over time and may require more equipment replacements.^{8,9} Further research should be done to quantify the degree of embrittlement and corrosion to assess costs associated with using carbon steel versus stainless steel. However, at the conceptual design phase we have assumed that despite the higher capital cost there will be sufficient savings on maintenance and replacement. Consequently, the decision was made to use stainless steel for nearly all process equipment. Some exceptions include storage tanks for water and diethyl ether which can be constructed out of carbon steel.

5. Health, Safety, and Environmental (HSE) Considerations

The most concerning hazard associated with the proposed process design is the flammability of the materials. In the proposed process, the materials will be at temperatures above 13°C, yet the flash points of ethanol, ethyl acetate, and diethyl ether are all at or below 13°C.^{10,11,12,13} Consequently, it is crucial that no ignition sources are present; including but not limited to open flames, faulty electrical equipment, and hot surfaces. To minimize the probability of an explosion, all parking lots should be located a safe distance from the plant. Further, all electrical equipment should be properly insulated or contained to reduce the chance of electrical sparks.

The reactor operates at 240°C and diethyl ether has the lowest auto-ignition temperature of 175°C. The lower explosive limit (LEL) of all flammable materials is less than or equal to 4% by volume. In the event of a leak at temperatures above 175°C, such as at the reactor effluent, diethyl ether would be exposed to oxygen from the ambient air. Thus, all leaks should be treated as an emergency event. It's recommended that a safety containment system be explored near the reactor to prevent an explosion should a leak occur. Any equipment used to transport or store materials should be installed in a cool, well-ventilated location and material should be stored under an inert gas.

Since reactions 1 and 2 are endothermic and produce temperature drops across the reactor, an explosion due to a runaway reaction is not of concern. However, the reactor inlet temperature is a crucial parameter to control, as it will affect all other downstream temperatures. Due to this, it is recommended that an emergency cooling system be installed at the reactor inlet to ensure the temperature is at or below 240°C.

To prevent pressure rises near the equipment's max pressure rating, especially in the high-pressure distillation columns, pressure relief valves and/or rupture disks should be installed on the reactor, inlet piping, and outlet piping. All pressure relief systems should direct chemicals to a flare tower and be back-filled with an inert gas to prevent oxygen from interacting with the flammable chemicals. Pumps and piping are inexpensive yet failures such as ruptures leading to toxic leaks can be catastrophic. Therefore, redundancy should be used when installing pumps and each pump should be equipped with a trip switch. Furthermore, all equipment should be equipped with alarms to alert operators of unsafe conditions such as unclosed mass balances, abnormal temperature rises, and pressures near the max pressure ratings of the equipment.

In addition to catastrophic failures such as gas leaks and explosions, general health and environmental concerns must be considered as well. The chemicals in our reaction are all toxic; ethyl acetate is an irritant and both ethyl acetate and diethyl ether cause dizziness and drowsiness following acute exposure. Proper safety equipment should always be worn when handling these chemicals and safety data sheets (SDSs) should be located wherever chemicals are handled. Any waste material should be properly stored in well labeled containers to be properly disposed of in a timely manner.

6. Important Considerations

6.1 Process Alternatives

While the current design has been chosen based on its practicality, economics, and safety, there are other possible design decisions that may prove to be good alternatives. One example is to use a reactive distillation unit to begin the separation. This has a lot of potential to break the azeotropes present in the multicomponent mixture as well as to decrease total equipment costs.¹³ Another possible alternative is to use nickel or zinc plating on process equipment to prevent hydrogen embrittlement. Depending on the unit operation, this may save maintenance costs while increasing the upfront installed cost. This would most likely only be recommended on flash separation unit where a high concentration of hydrogen is present.

The current design uses a pressure swing adsorption system to break the ethanol-water azeotrope and recycle the residual ethyl acetate in the ethanol stream. This PSA unit could be replaced with distillation columns and the addition of an entrainer to break the azeotrope. Other liquid adsorption columns could also prove to be effective separation units for this split.

The final important process alternative is the currently absent diethyl ether separation system. This may be liquid extraction design or a column with an adsorbent. If the diethyl ether were to be separated via distillation, the distillation space would gain one dimension and the residue curve map would become a tetrahedron, complicating the distillation.

6.2 Future Experimentation

A very important piece of the feasibility of this design is the vapor liquid equilibrium in the multicomponent separation. There are several azeotropes that vary or disappear as the pressure is adjusted, and the separation system design is very sensitive to small changes in the feed stream composition as well as the equilibrium data. Therefore, it is very important that the fluid models used to simulate the distillation are correct. UNIQUAC was used for the designs in this report, but when changing the model to UNIFAC or NRTL, there are differences in the residue curve map which could affect the design. Because of this, it is recommended that vapor liquid equilibrium experiments are carried out to verify the models before these designs are implemented.

Catalyst life can also be tested to determine if the rate of catalyst deactivation requires further analysis. At the current catalyst cost, if a larger reactor is needed, needing to replace the catalyst less frequently could save on operating costs. Furthermore, the reactor volume is in doubt, and based on the high economic implications of an incorrect reactor volume, the kinetics for this reaction set should be confirmed.

6.3 Ethical and Professional Considerations

Major project delays such as a strike among the union workers can have a profound effect on completion of construction. Economically the plant will be unable to begin producing a revenue stream for the company but added cost may arise from postponing certain stages in the construction process. To avoid such action management may attempt to break the strike with methods that require ethical consideration.

Ideally a discussion with the union leaders and coming to a resolution is the most optimal outcome. Coming to an agreeable resolution may not be a quick process. Alternatively, non-union workers may be brought in to continue work while discussions with union workers continue. While this attempts to minimize the damage from the union strike, the replacement workers may be more expensive than budgeted with union work. There exists the potential for the non-union workers to eventually join the union. Bringing in a foreign team to replace the union strikers will hinder any negotiations with the current union strike. Issues with the foreign workers may arise from poor communication or different business practices. A third strategy is to negotiate with individual union members to return to work despite the ongoing strike. One could anticipate the performance and skills of these workers, but it would be unlikely to attain a complete workforce with this strategy.

7. Conclusions

This design focused on maximizing NPV% while also placing considerable weight on safety, carbon emissions, and feasibility. Based on the robust potential for returns on this investment, the techno-economic analysis should be further investigated. With an ROI_{BT} of 14%, the sales revenue from this process is highly profitable relative to the required capital investment of \$35 MM. The market shock, construction delay, and excess cost simulations indicate the manageable risk associated with this venture. More accurate cost estimates and ethyl acetate price data should be pursued to further improve the estimates of plant profitability.

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9. Appendices

9.1 Appendix A: Figures

Appendix A.1: Conceptual Design Figures

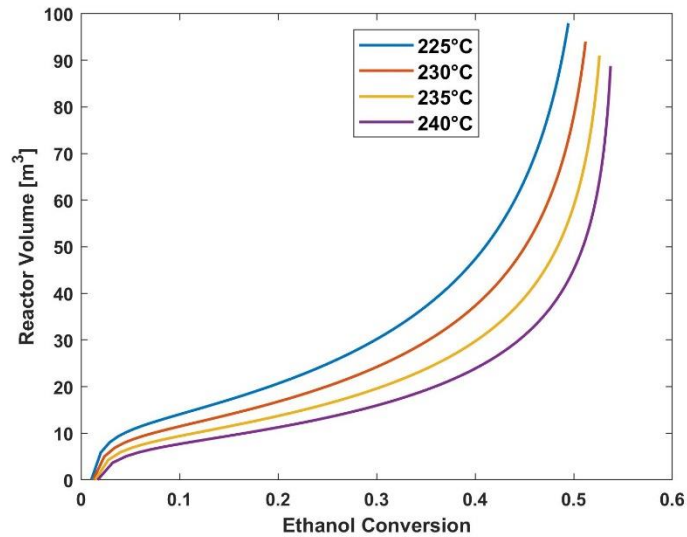


Figure A.1.1. Reactor volume as a function of single pass toluene conversion for multiple temperatures. Increasing reactor temperature significantly reduces the reactor volume required to achieve a desired conversion.

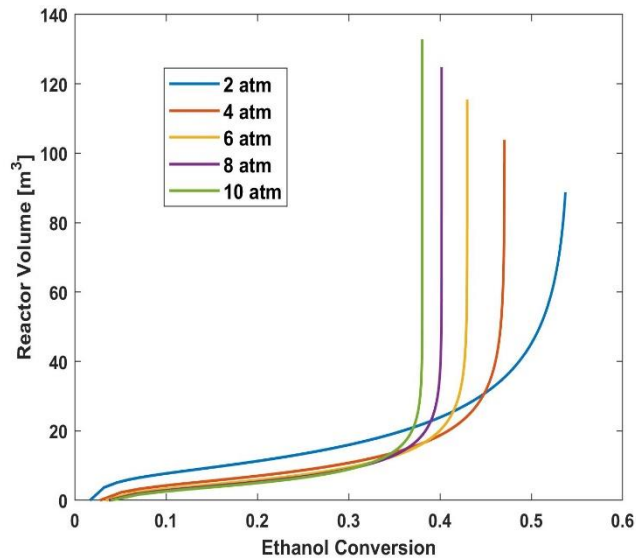


Figure A.1.2. Reactor volume as a function of single pass toluene conversion for multiple pressures. Increasing reactor pressure reduces the reactor volume required to achieve a desired conversion at low conversions, then it reverses at higher conversions.

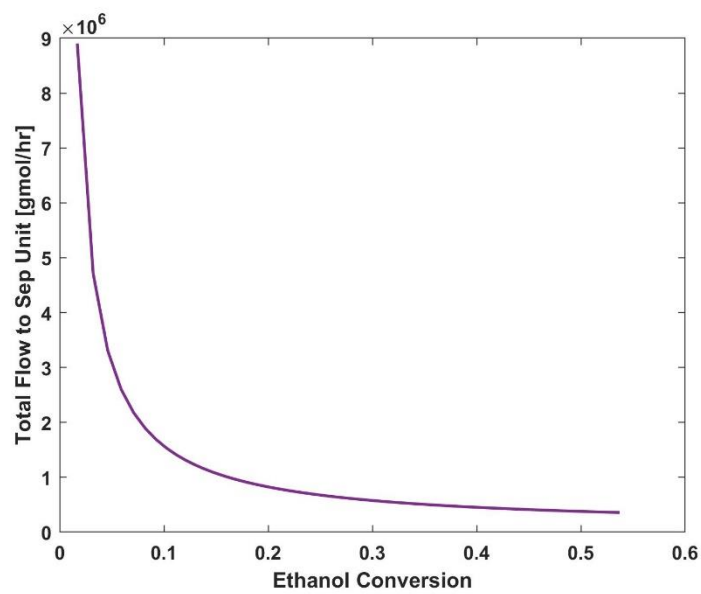


Figure A.1.3. Total molar flow to the separations unit as a function of reactor conversion

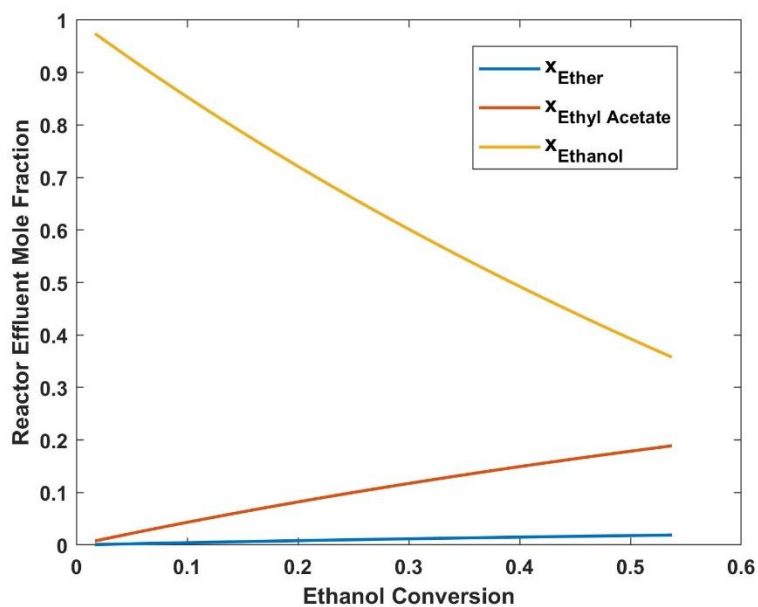


Figure A.1.4. Mole fraction of components entering separation system as a function of reactor conversion. Water mole fraction is equivalent to ether mole fraction.

Appendix A.2: Economics Figures

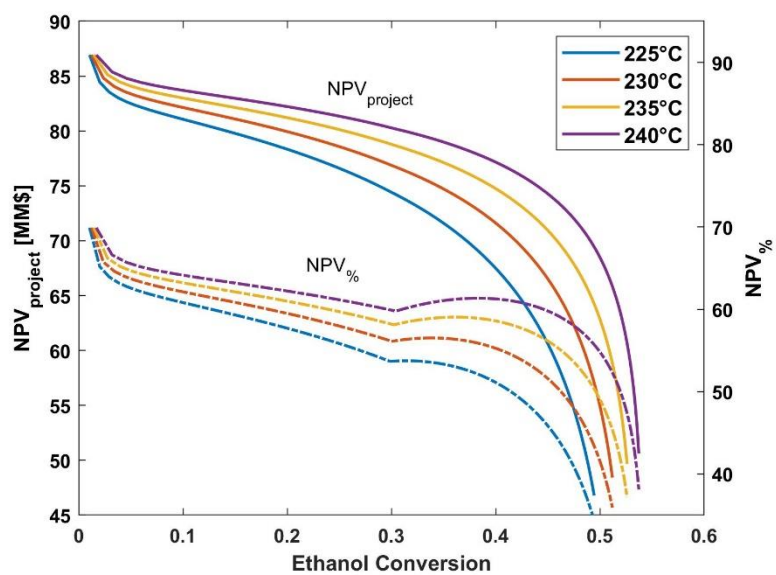


Figure A.2.1. NPV as a function of reactor conversion at various reactor temperatures without any separations system

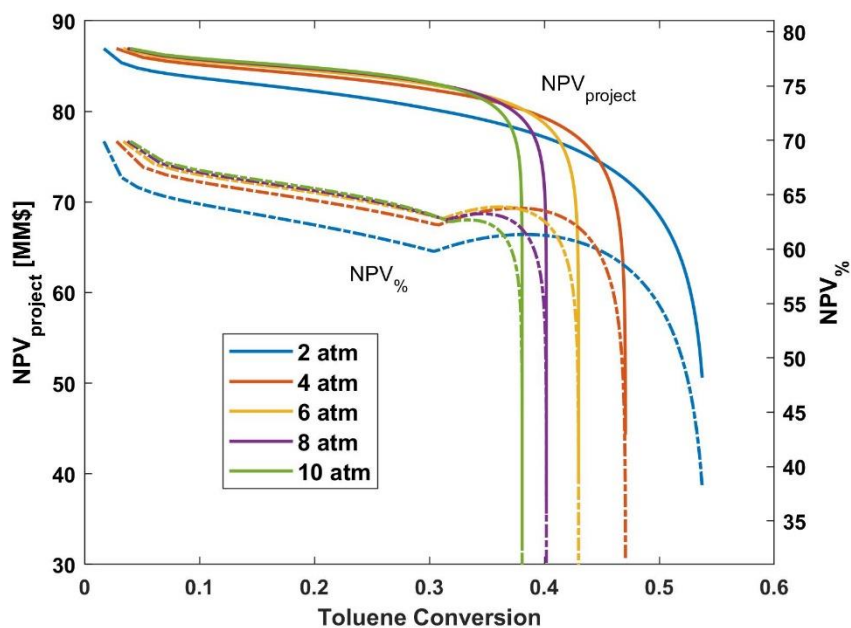


Figure A.2.2. Total Capital Investment (TCI) as a function of reactor conversion. High reactor conversion decreases the required size of the equipment and separations system capital cost

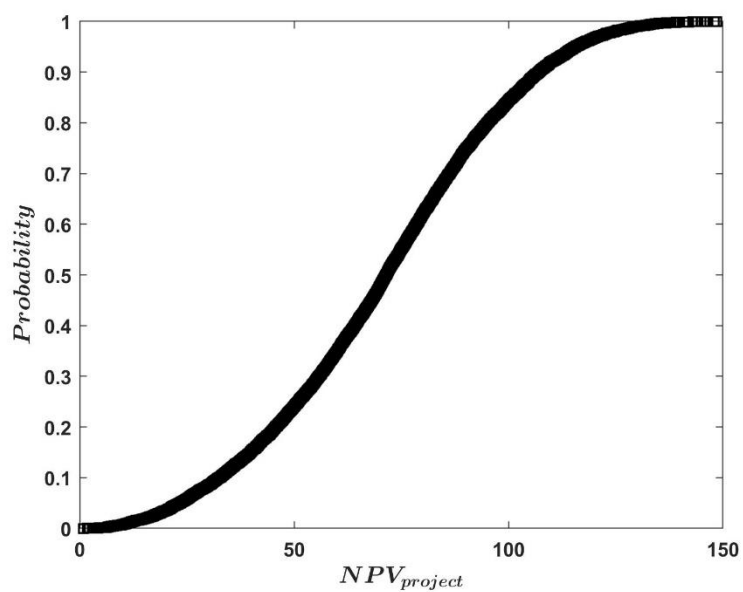


Figure A.2.3. Cumulative distribution function of $NPV_{project}$ for Monte Carlo simulation with 10,000 randomized trials of economic parameters.

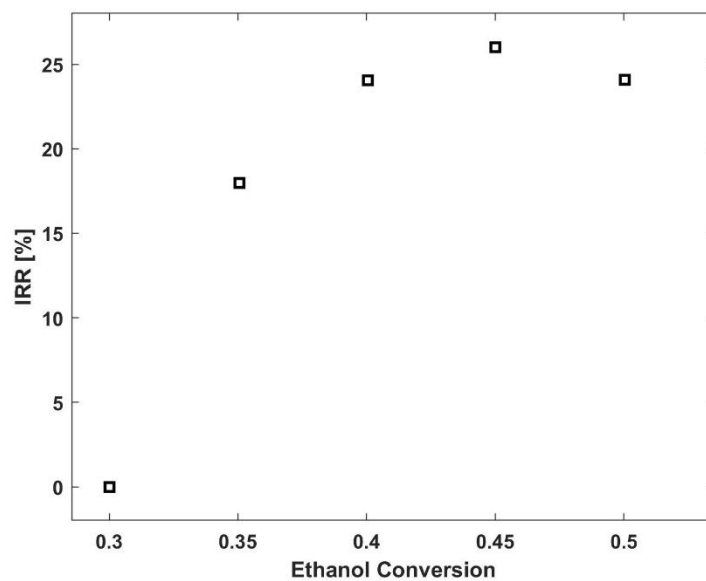


Figure A.2.4. IRR is optimized at 45% conversion, 2 atm, and 240°C

9.2 Appendix B: Economic Analysis

Revenue (R) = \$55 MM/year

Ethyl Acetate Sales:

$$50,000 \text{ MT} \frac{\text{ethyl acetate}}{\text{year}} \times \frac{\$1,100}{\text{MT ethyl acetate}} = \$55 \text{ MM/year}$$

Cost (C) = \$ 40.2 MM/year

Raw Ethanol:

$$59,314 \frac{\text{MT ethanol}}{\text{year}} \times \frac{\$500}{\text{MT ethanol}} = \$29.8 \text{ MM/year}$$

Separations System Operation:

$$\$1.97 \text{ MM/year}$$

Heat Exchanger Steam:

$$\$0.39 \text{ MM/year}$$

Heat Exchanger Coolant:

$$\$1.25 \text{ MM/year}$$

Carbon Tax:

$$935 \frac{\text{MT CO}_2}{\text{year}} \times \frac{\$40}{\text{MT}} = \$0.37 \text{ MM/year}$$

Administration and General Services:

$$0.1 \times R = \$5.5 \text{ MM/year}$$

Replacement Catalyst (cost averaged over 6-month lifetime):

$$50.5 \frac{\text{MT catalyst}}{\text{year}} \times \frac{\$10,000}{\text{MT catalyst}} = \$0.51 \text{ MM/year}$$

Profit Before Taxes (P_{BT}) = \$14.8 MM/year

$$P_{BT} = R - C = \$14.8 \text{ MM/year}$$

ISBL (Installed Cost) = \$7.3 MM

Equipment Cost Correlations¹⁴

Reactor

$$\text{InstalledCost}[\$] = \left(\frac{M\&S}{280} \right) (101.9 D^{1.066} H^{0.82} F_c) = \$0.22 \text{ MM} \quad [5]$$

$D = \text{Diameter, ft}$
 $H = \text{Height, ft}$
 $F_c = F_m F_p$
 For Carbon Reactor, $F_m = 3.75$
 For less than 200 psi, $F_p = 1$

Heat Exchangers

$$\text{InstalledCost}[\$] = \left(\frac{M\&S}{280} \right) (101.3 A^{0.65}) F_c \quad [3]$$

$F_c = (F_d + F_p) F_m$
 For Fixed – tube – sheet, $F_d = 0.8$
 For Titanium, $F_m = 8.95$

For Stainless Steel, $F_m = 3.75$
For Carbon Steel, $F_m = 1.0$
For less than 150 psi, $F_p = 0$
For less than 800 psi, $F_p = 0.52$

Heat Exchanger	U [Btu/F ft ² h]	Q [MW]	Area [ft ²]	Material	Pressure [psi]	Cost [\$]
E-100	17.6	0.99	1,110	SS	66	312,000
E-101	146	3.17	594	SS	147	231,000
E-102	19.4	1.20	2,023	Ti	735	393,000
E-103	136	4.08	1,404	SS	15	657,000
E-104	141	0.63	116	SS	15	65,000
E-105	141	0.01	4	SS	15	6,000

Distillation Columns

$$\text{Installed Cost } [\$] = \left(\frac{M\&S}{310} \right) (5000) (F_c + 5) \left(\frac{D}{3.28} \right) \left(\frac{H}{20} \right)^{0.82}$$

D = Column Diameter, ft
 H = Column Height, ft
 $F_c = F_m F_p$
For Carbon Steel, $F_m = 1.0$
For up to 200 psi, $F_p = 1.15$
For up to 300 psi, $F_p = 1.2$

Distillation Column Internals

$$\text{Installed Cost } [\$] = \left(\frac{M\&S}{301} \right) (F_{c,t}) 500 \left(\frac{H}{20} \right) \left(\frac{D}{3.28} \right)^{1.8}$$

D = Column Diameter, ft
 H = tray stack height, ft (24 – in. spacing)
 $F_c = F_s + F_t + F_m$
For 24 in. tray spacing, $F_s = 1.0$
For sieve type trays, $F_t = 0.0$
For carbon steel trays, $F_m = 0.0$

Column	Height [ft]	Diameter [ft]	Trays	Pressure [psi]	Material	Operating Cost [\$ /yr]	Cost [\$]
T-100	56	8	28	15	SS	970,000	2,130,000
T-101	86	6	43	294	SS	910,000	2,910,000
V-100	16	3	0	22	SS	0	114,000

Working Capital (WC) = \$8.3 MM

$$2 \text{ month } \times \frac{59,500 \text{ MT toluene}}{\text{year}} \times \frac{1 \text{ year}}{12 \text{ months}} \times \frac{\$500}{\text{MT toluene}} = \$ 5.0 \text{ MM}$$

Total Capital Investment (TCI) = \$35 MM

$$TCI = 1.3 \times 1.4 \times 2 \times (FCI + SU) + WC = \$ 35 \text{ MM}$$

Year	Construction Period							Discount Factors	DCF
-2	Fixed Capital	0				Construction Rate	5%	1.103	0
-1	Fixed Capital	-15,952,067	TCI	35,002,559	Finance Rate	3%		1.050	-16,749,670
0	Fixed Capital	-10,634,711	Profit_BT	14,435,773	Tax Rate	27%		1.000	-10,634,711
0	Working Capital	-4,959,500	ROI_BT	41.2%	Enterprise Rate	10%		1.000	-4,959,500
0	Start-Up Capital	-2,658,678				N _{Construction}	2	1.000	-2,658,678
						N _{operations}	15		-35,002,559
	Operations Period		Profit Before Taxes	Bond Financing	Depreciation Allowed	Profit After Taxes	Cash Flow	Discount Factors	DCF
1	Pay-Off TCI		7,217,887	-1,050,077	2,897,959	2,386,991	5,284,950	0.909	4,804,500
2			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.826	8,722,320
3			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.751	7,929,382
4			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.683	7,208,529
5			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.621	6,553,208
6			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.564	5,957,462
7			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.513	5,415,874
8			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.467	4,923,522
9			14,435,773	-1,050,077	2,897,959	7,656,048	10,554,007	0.424	4,475,929
10			14,435,773	-1,050,077	2,897,959	7,656,048	7,656,048	0.386	2,951,738
10				-35,002,559			-35,002,559	0.386	-13,495,002
11	Working Capital		14,435,773			10,538,114	10,538,114	0.350	3,693,545
12			14,435,773			10,538,114	10,538,114	0.319	3,357,768
13			14,435,773			10,538,114	10,538,114	0.290	3,052,516
14			14,435,773			10,538,114	10,538,114	0.263	2,775,015
15			14,435,773			10,538,114	10,538,114	0.239	2,522,741
15	Working Capital	4,959,500					4,959,500	0.239	1,187,265
15	Salvage Value	265,868					265,868	0.239	63,647
								NPV_%	NPV
								8.6%	51,322,281

Figure B.1. Cash flow sheet with NPV and NPV% calculations

Year	Construction Period							Discount Factors	DCF
-2	Fixed Capital	0			Construction Rate		5%	1.520	0
-1	Fixed Capital	-15,952,067	TCI	37,917,979	Finance Rate		3%	1.233	-19,665,090
0	Fixed Capital	-10,634,711	Profit_BT	14,435,773	Tax Rate		27%	1.000	-10,634,711
0	Working Capital	-4,959,500	ROI_BT	38.1%	Enterprise Rate		10%	1.000	-4,959,500
0	Start-Up Capital	-2,658,678			N _{Construction}		2	1.000	-2,658,678
					N _{operations}		15		-37,917,979
	Operations Period		Profit Before Taxes	Bond Financing	Depreciation Allowed	Profit After Taxes	Cash Flow	Discount Factors	DCF
1	Pay-Off TCI		7,217,887	-37,917,979	2,897,959	3,153,547	6,051,506	0.811	4,908,904
2			14,435,773		2,897,959	8,422,604	11,320,563	0.658	7,449,208
3			14,435,773		2,897,959	8,422,604	11,320,563	0.534	6,042,701
4			14,435,773		2,897,959	8,422,604	11,320,563	0.433	4,901,761
5			14,435,773		2,897,959	8,422,604	11,320,563	0.351	3,976,245
6			14,435,773		2,897,959	8,422,604	11,320,563	0.285	3,225,479
7			14,435,773		2,897,959	8,422,604	11,320,563	0.231	2,616,467
8			14,435,773		2,897,959	8,422,604	11,320,563	0.187	2,122,444
9			14,435,773		2,897,959	8,422,604	11,320,563	0.152	1,721,699
10			14,435,773		2,897,959	14,435,773	14,435,773	0.123	1,780,944
10						-37,917,979	0.123	-4,677,948	
11			14,435,773			10,538,114	10,538,114	0.100	1,054,616
12			14,435,773			10,538,114	10,538,114	0.081	855,490
13			14,435,773			10,538,114	10,538,114	0.066	693,963
14			14,435,773			10,538,114	10,538,114	0.053	562,934
15			14,435,773			10,538,114	10,538,114	0.043	456,645
15	Working Capital	4,959,500					4,959,500	0.043	214,908
15	Salvage Value	265,868					265,868	0.043	11,521
								IRR	NPV
								23.3%	0

Figure B.2. Cash flow sheet with IRR calculation

9.3 Appendix C: Chemical Physical Properties and Health and Safety Information

Table C.1 Chemical properties

	Ethanol	Acetaldehyde	Hydrogen Gas	Ethyl Acetate	Diethyl Ether	Water
Molecular Weight [g/mol]	46.07	44.05	2.02	88.11	74.12	18.02
Heat Capacity (C_p) [kJ/kgmol-°C]	120.7	-	30.2	178.2	175.6	74.6
Heat Capacity (C_v) [kJ/kgmol-°C]	112.4	-	21.9	169.9	175.4	66.2
Liquid Density [kg/m³]	789	780	-	902	710	1000
Heat of Vaporization [kJ/mol]	38.6	25.76	0.45	31.94	29	40.65
Molar Volume [m³/kgmol]	0.058	-	14.99	0.099	0.28	0.018
Auto-ignition Temperature [°C]	455	175	536	427	175	-
Flash Point [°C]	13	-38.89	-150	-4	-40	-
Melting Point [°C]	-114	-123.5	-259.2	-83.6	-116	0
Initial Boiling Point [°C]	78	21	-252.8	76.5	34.6	100
Upper Explosive Limit [%V]	14	57	75	12	36	-
Lower Explosive Limit [%V]	3	4	4	2	2	-

Table C.2 Chemical Hazards and Toxicology

Species	Hazards	Toxicology
Ethanol	Highly flammable liquid and vapor	LD50 Oral (rat) - 10,470 mg/kg
Acetaldehyde	Highly flammable liquid and vapor Causes skin eye and respiratory irritation May cause cancer	LD50 Oral (rat) - 661 mg/kg
Hydrogen Gas	Highly flammable vapor	No LD50 Data
Ethyl Acetate	Highly flammable liquid and vapor Causes eye irritation May cause drowsiness or dizziness	LD50 Oral (rat) - 5,620 mg/kg
Diethyl Ether	Highly flammable liquid and vapor Harmful if swallowed May cause drowsiness or dizziness	LD50 Oral (rat) -1,211 mg/kg
Water	Not a hazardous substance	LD50 Oral (rat) - 90,000 mg/kg

Table C.3 HAZOP Analysis

Sources of Hazard	Incidents	Hazard	Consequence
Diethyl Ether near Reactor Effluent	Leak	Fire/Explosion	Injury/damage
Diethyl Ether, Ethyl Acetate, Ethanol, Hydrogen Transportation	Leak and Ignition	Fire/Explosion	Injury/damage
Diethyl Ether, Ethyl Acetate, Ethanol, Hydrogen Storage	Leak and Ignition	Fire/Explosion	Injury/damage
Diethyl Ether, Ethyl Acetate, Ethanol, Hydrogen Transportation	Leak	Inhalation/Dermal Contact	Irritation/Asphyxiation
Diethyl Ether, Ethyl Acetate, Ethanol, Hydrogen Storage	Leak	Inhalation/Dermal Contact	Irritation/Asphyxiation

9.4 Appendix D: Molar Material Balances and Split Decisions

Level 2

The most general mole balance on all components entering, reacting, and exiting out plant yields equation 1

$$\begin{bmatrix} F_E \\ F_{EA} \\ F_{DE} \\ F_W \\ F_H \end{bmatrix} - \begin{bmatrix} P_E \\ P_{EA} \\ P_{DE} \\ P_W \\ P_H \end{bmatrix} + \begin{bmatrix} -2 & -2 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 2 & 0 \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad [1]$$

At level 2, we are recycling all ethanol internally and we do not feed any ethyl acetate, diethyl ether, water, or hydrogen to our plant. This reduces the system to:

$$\begin{bmatrix} F_E \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ P_{EA} \\ P_{DE} \\ P_W \\ P_H \end{bmatrix} + \begin{bmatrix} -2 & -2 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 2 & 0 \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad [2]$$

We then solve for hydrogen and water as our reference components

$$-1/2 P_H + \xi_1 = 0 \quad [3]$$

$$-P_W + \xi_2 = 0 \quad [4]$$

We then can make a substitution into our system of non-reference components:

$$F_E - P_H - 2P_W = 0 \quad [5]$$

$$-P_{EA} + 1/2 P_H = 0 \quad [6]$$

$$P_W - P_{DE} = 0 \quad [7]$$

Specifications:

$$P_{EA} = 50 \text{ kta}$$

$$\xi_2 = \frac{1}{10} \xi_1 \text{ equivalently, } P_W = \frac{1}{20} P_H$$

Substituting these specifications into our non-reference moles balances and rearranging results in the following equivalently

$$P_W = P_{DE} = \frac{11}{10} P_{EA} - P_{EA} = \frac{1}{10} P_{EA} \quad [8]$$

$$P_H = 20 P_W = 2 P_{EA} \quad [9]$$

$$F_E = 2 P_{EA} + \frac{1}{5} P_{EA} = \frac{11}{5} P_{EA} \quad [10]$$

Level 3

From our level 2 mole balances, we have determined the feed rate of ethanol to the reactor and the flowrate of ethyl acetate, diethyl ether, water, and hydrogen leaving the separation system. At Level 3 a recycle stream is introduced to our process to return all ethanol in the reactor effluent to the reactor feed stream. Performing a mole balance on the fresh feed and recycle mixer produces the following.

$$F_{FE} + R_E = F_E \quad [11]$$

x_E is the per pass reactor toluene conversion defined as

$$x_E = \frac{F_E - R_E}{F_E} \quad [12]$$

The rearranging this for R_E yields

$$R_E = (1 - x_E)F_E \quad [13]$$

Substituting this relation into our mixer mole balance determines the required fresh feed of toluene to the plant.

$$F_{FE} = F_E - R_E = x_E F_E \quad [14]$$

Stating the fresh plant feed and recycle molar flowrates in terms of the design specifications yield the following.

$$R_E = \frac{11}{5} P_{EA} (1 - x_E) \quad [15]$$

$$F_{FE} = \frac{11}{5} x_E P_{EA} \quad [16]$$

Aspen Plus Residue Curves

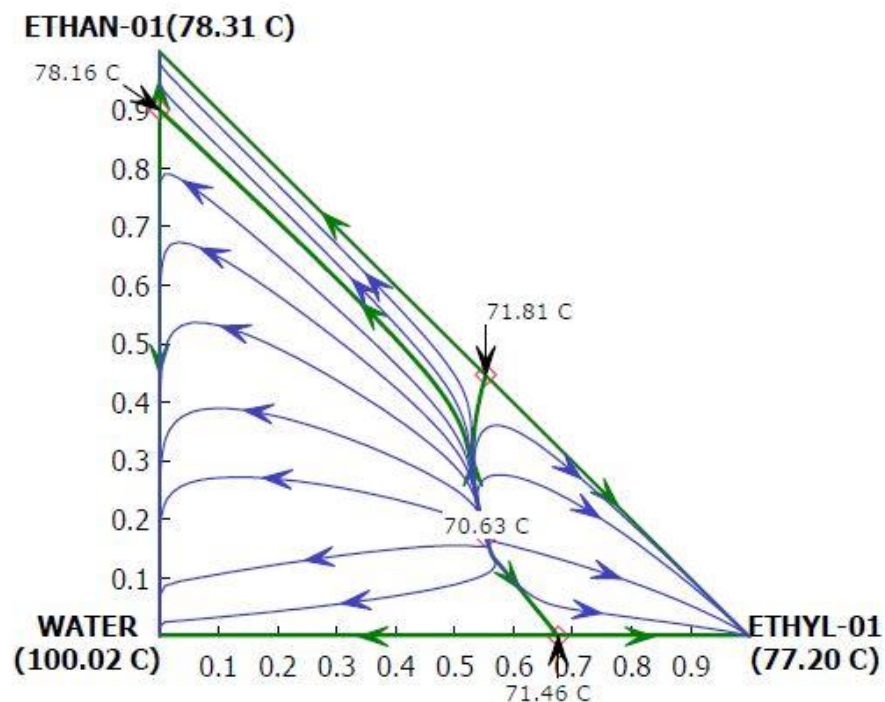


Figure 1. Water, ethanol, and ethyl acetate residue curve at 1 atm

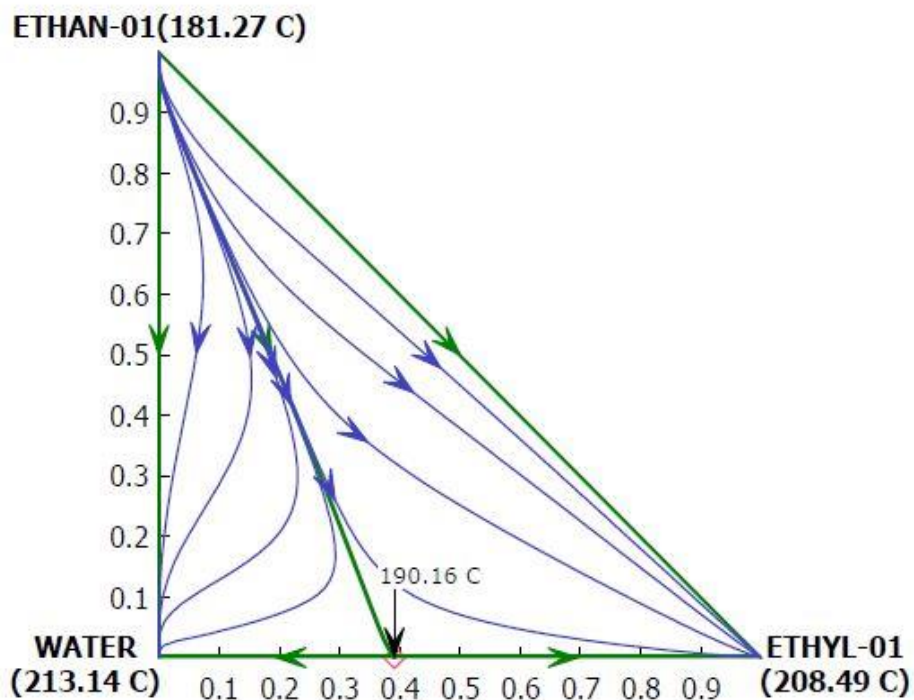


Figure 2. Water, ethanol, and ethyl acetate residue curve at 20 atm

9.5 Appendix E: Stream Table

Process Stream	Feed - 01	Product - 01	Product - 02	Product - 03	Product - 04	Recycle - 01
Description	Ethanol Fresh Feed	Ethyl Acetate Product	Hydrogen for Steam Generation	Diethyl Ether for Steam generation	Water Product	X - 101 PSA Ethanol Output
Flow Rate [kg/hr]	7085	5952	533.4	468.6	123.9	8875
Flow Rate [MT/year]	59514	49997	4480.56	3936.24	1040.76	74550
Temperature [°C]	25	30	1	2.2	30	77.54
Pressure [kPa]	101.3	101.3	152	152	101.3	101.3
Vapor Fraction	0	0	1	0.0121	0	0
Water Mole Fraction	0	0	0.0004	0	1	0
Diethyl Ether Mole Fraction	0	0	0.0043	0.9899	0	0
Ethanol Mole Fraction	1	0	0.0085	0	0	0.9763
Hydrogen Mole Fraction	0	0	0.9747	0.0101	0	0
Ethyl Acetate	0	1	0.0122	0	0	0.0237

Process Stream	Stream - 01	Stream - 02	Stream - 03	Stream - 04	Stream - 05	Stream - 06
Description	Mixed Ethanol Pump Inlet	Ethanol Feed to HX Series	Ethanol Feed E - 100 to E - 101	Ethanol Feed E - 101 to E - 102	Reactor Feed	Reactor Outlet
Flow Rate [kg/hr]	15950	15950	15950	15950	15950	15950
Flow Rate [MT/year]	133980	133980	133980	133980	133980	133980
Temperature [°C]	55.33	55.54	122	96.85	240	240
Pressure [kPa]	101.3	456	456	202.6	202.6	192.6
Vapor Fraction	0	0	0	1	1	1
Water Mole Fraction	0	0	0	0	0	0.0168
Diethyl Ether Mole Fraction	0	0	0	0	0	0.0168
Ethanol Mole Fraction	0.9869	0.9869	0.9869	0.9869	0.9869	0.4503
Hydrogen Mole Fraction	0	0	0	0	0	0.3367
Ethyl Acetate	0.0131	0.0131	0.0131	0.0131	0.0131	0.1792

Process Stream	Stream - 07	Stream - 08	Stream - 09	Stream - 10	Stream - 11	Stream - 12
Description	Effluent E - 100 to E - 103	Cooled Effluent to Hydrogen Flash	Flash Bottoms	Diethyl Ether Split Block Bottoms	T - 100 Bottoms to Mixer	T - 100 Distillate to P - 100
Flow Rate [kg/hr]	15950	15950	15420	14950	5680	9271
Flow Rate [MT/year]	133980	133980	129528	125580	47712	77876.4
Temperature [°C]	132.9	2.1	1	84.21	78.27	71.52
Pressure [kPa]	192.6	152	152	152	101.3	101.3
Vapor Fraction	1	0.346	0	0	0	0
Water Mole Fraction	0.0168	0.0168	0.0255	0.0261	0.0141	0.0369
Diethyl Ether Mole Fraction	0.0168	0.0168	0.0235	0	0	0
Ethanol Mole Fraction	0.4503	0.4503	0.6834	0.7	0.9859	0.4435
Hydrogen Mole Fraction	0.3367	0.3367	0.0002	0	0	0
Ethyl Acetate	0.1792	0.1792	0.2674	0.2739	0	0.5196

Process Stream	Stream - 13	Stream - 14	Stream - 15	Stream - 16	Stream - 17	Stream - 18	Stream - 19
Description	Pressurized Feed to T - 101	T - 101 Ethanol Distillate to Valve	T - 101 Low Pressure Distillate to Mixer	T - 101 Ethyl Acetate Bottoms	Cooled Ethyl Acetate	Ethanol and Water mixture to PSA unit	PSA Water outlet
Flow Rate [kg/hr]	9271	3319	3319	5952	5952	8999	123.9
Flow Rate [MT/year]	77876.4	27879.6	27879.6	49996.8	49996.8	75591.6	1040.76
Temperature [°C]	72.76	181.7	76.88	208.5	70	77.6	100
Pressure [kPa]	2026	2026	101.3	2026	2026	101.3	101.3
Vapor Fraction	0	0	0	0	0	0.192	0
Water Mole Fraction	0.0369	0.072	0.072	0	0	0.0352	1
Diethyl Ether Mole Fraction	0	0	0	0	0	0	0
Ethanol Mole Fraction	0.4435	0.865	0.865	0	0	0.9419	0
Hydrogen Mole Fraction	0	0	0	0	0	0	0
Ethyl Acetate	0.5196	0.063	0.063	1	1	0.0229	0

Utility Stream	Steam - 01	Condensate - 01	Steam - 02	Condensate - 02
Description	Steam Feed to E - 102	Condensed Steam from E - 102	Steam Feed to E - 102	Condensed Steam from E - 102
Flow Rate [kg/hr]	5644	5644	2161	2161
Flow Rate [MT/year]	47409.6	47409.6	18152.4	18152.4
Temperature [°C]	180	180	264.8	210
Pressure [kPa]	1000	1000	5066	5066
Vapor Fraction	1	0	1	0

Unit Operation	E - 100	E - 101	E - 102	E - 103	E - 104	E - 105
Description	Process Fluid Integrated Heat Exchanger	Steam Kettle Reboiler	Steam Heat Exchanger	Separation Pre-Cooler	Ethyl Acetate Cooler	Water Cooler
Material	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Carbon Steel	Carbon Steel
Duty [MW]	0.992	3.156	1.204	4.072	0.764	0.010
Installed Cost [\$ MM]	0.31	0.23	0.39	0.66	0.06	0.01
Operating Cost [\$ MM/yr]	-	0.25	0.13	1.19	0.06	0.001

Unit Operation	PFR - 100	T-100	T-101	V-100	X-100	X-101
Description	Packed Bed Reactor	First Distillation Column	Second Distillation Column	Hydrogen Flash Drum	Diethyl Ether Separation Unit	Water/Ethanol PSA Separation Unit
Volume [m ³]	8.0	87.4	78.4	3.3	-	-
Temperature [°C]	240	71.5-78.3	181.8-202.7	1	-	-
Pressure [atm]	2	1	20	1.5	-	-
Conversion [%]	45	-	-	-	-	-
Material and Catalyst	Stainless Steel 94:5:1 CuO:CoO:Cr ₂ O ₃	Stainless Steel	Stainless Steel	Stainless Steel	-	Carbon Steel
Feed Rate [kg/hr]	15950	14950	9271	15950	15420	8999
Feed Rate [MT/yr]	133980	125580	77876	133980	129528	75592
Vapor Flow Rate [kg/hr]	-	51285	57115	533.4	-	-
V/F [kg/kg]	-	3.430	6.161	-	-	-
Number of Trays	-	28	43	-	-	-
Reboiler Ratio	-	6.8	14.7	-	-	-
Reflux ratio	-	6	7	-	-	-
Duty [MW]	0.585	9.306 [Condenser] 9.167 [Reboiler]	4.222 [Condenser] 5.131 [Reboiler]	16.397	-	-
Installed Cost [\$ MM]	0.23	2.12	2.92	0.11	0.016	0.917
Operating Cost [\$ MM/yr]	0.47	0.97	0.91	-	-	-

9.6 Appendix F: HYSYS vs MATLAB Comparison

Design Parameter	MATLAB	HYSYS	Units
Fresh Feed Ethanol			
Mass Flowrate	6.85	7.09	MT /h
Temperature	N/A	25	C
Pressure	N/A	1.0	atm
Reactor Specification			
Reactor Assumptions	Isothermal No Pressure Drop	Isothermal Fixed Pressure drop	-
Reactor Volume	31.1	8	m ³
Void Fraction	0.5	0.5	-
Void Volume	15.6	4	m ³
Tube Count	1	1	-
Tube Diameter	1.7	1.01	m
Tube Length	17	10	m
Temperature	240	240	C
Total Pressure	2	2	atm
Single Pass Ethanol Conversion	0.451	0.451	-
Reactor Inlet Conditions			
Temperature	240	240	C
Pressure	2	2	atm
Total Mass Flowrate	15.2	15.95	MT/h
Fresh Ethanol Mass Flowrate	6.85	7.09	MT /h
Recycled Ethanol Mass Flowrate	8.35	8.47	MT /h

Reactor Outlet Conditions			
Temperature	240	240	C
Pressure	2	1.5	atm
Total Mass Flowrate	15.2	15.95	MT /h
Mass Flowrate of Ethyl Acetate	5.95	6.50	MT /h
Mass Flowrate of Ethanol	8.35	8.54	MT /h
Mass Flowrate of Hydrogen	0.3	0.28	MT /h
Mass Flowrate of Water	0.12	0.12	MT /h
Distillation Column Parameters			
	Aspen Plus	HYSYS	
T-101 Pressure	20	20	atm
T-100 Pressure	1	1	atm
T - 101 Number of Stages	43.1	43	-
T - 100 Number of Stages	27.8	28	-
T - 101 Reflux Ratio	7	7	-
T - 100 Reflux Ratio	6	6	-
T - 101 Reboiler Ratio	9.53	14.7	-
T - 100 Reboiler Ratio	6.78	6.77	-
T - 101 Diameter	-	1.95	m
T - 100 Diameter	-	2.55	m
T - 101 Height	-	26.2	m
T - 100 Height	-	17.1	m

9.7 Appendix G: Team Member Work Statements

Team Member Work Statement

Brad Kooker

I wrote the code for modeling the PFR for various temperatures and implemented Matt's level 3 mole balances to calculate all molar flowrates through the plant. I performed the HYSYS simulation. I also performed the distillation design in Aspen Plus with insight from Matt and John. In writing the report I primarily contributed to the writing of the Aspen HYSYS Simulation and ethical considerations regarding a union strike. I also contributed to the writing of the calculations in the appendices.

John Gelinas

I created the Conceptual Design MATLAB optimization code based on Brad's PFR code and base, including adding in the separations system numbers from Brad's aspen plus simulations. In addition, I performed the sensitivity analysis on the economic results, yielding the Tornado plot in excel and the Monte Carlo simulation in MATLAB. I created the Process Flow Diagram using Microsoft Visio based on the Hysys design. I also created the stream table and unit ops tables. I also created the figures in the report from these MATLAB scripts and excel files. I primarily contributed to writing the Conceptual Design Overview and Economic Analysis sections.

Matt Simmons

I created the excel cash flow spreadsheet and calculated economic profitability metrics (NPV, IRR, ROI_{BT} , NPV%). I made a table and pie chart summarizing equipment CAPEX and OPEX. I performed market shock and construction delay/excess cost analysis using the cash flow sheet. I performed the HAZOP analysis and tabulated the results. I created a cumulative cash flow diagram. For the report I contributed to writing the conceptual design, health and safety, materials of construction, and economic analysis sections.

Print Name and Sign: Brad Kooker
Bradley Kooker

Date: 6/2/20

Print Name and Sign: John Gelinas
John Gelinas

Date: 6/2/20

Print Name and Sign: Matt Simmons
Matt Simmons

Date: 6/2/20

Rating of Team Members for Design Project

Please rate each group member's contributions in the categories below:
 1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
 Each member fills out one form and signs the bottom.

Name :	1) Brad Kooker	2) John Gelinas	3) Matt Simmons
Quality of work presented	__5__	__5__	__5__
Quantity of work performed	__5__	__5__	__5__
Effort	__5__	__5__	__5__
Punctuality (meetings and deadlines)	__5__	__5__	__5__
Knowledge of design methods	__5__	__5__	__5__
Class attendance	__5__	__5__	__5__
Communication	__5__	__5__	__5__

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes

It's important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: Brad Kooker
Bradley Kooker

Date: 6/2/20

Rating of Team Members for Design Project

Please rate each group member's contributions in the categories below:

1-2 - unsatisfactory, 3 - acceptable/adequate, 4 - very good, 5 - excellent

Each member fills out one form and signs the bottom.

Name :	1) Brad Kooker	2) John Gelinas	3) Matt Simmons
Quality of work presented	__5__	__5__	__5__
Quantity of work performed	__5__	__5__	__5__
Effort	__5__	__5__	__5__
Punctuality (meetings and deadlines)	__5__	__5__	__5__
Knowledge of design methods	__5__	__5__	__5__
Class attendance	__5__	__5__	__5__
Communication	__5__	__5__	__5__

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes

It's important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: John Gelinas
John Gelinas

Date: 6/2/20

Rating of Team Members for Design Project

Please rate each group member's contributions in the categories below:

1-2 - unsatisfactory, 3 - acceptable/adequate, 4 - very good, 5 - excellent

Each member fills out one form and signs the bottom.

Name : 1) Brad Kooker 2) John Gelinas 3) Matt Simmons

Quality of work ___5___ ___5___ ___5___
presented

Quantity of work ___5___ ___5___ ___5___
performed

Effort ___5___ ___5___ ___5___

Punctuality ___5___ ___5___ ___5___
(meetings and
deadlines)

Knowledge of ___5___ ___5___ ___5___
design methods

Class attendance ___5___ ___5___ ___5___

Communication ___5___ ___5___ ___5___

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes

It's important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: Matt Simmons
Matt Simmons

Date: 6/2/20

9.8 Appendix H: MATLAB Code

MATLAB Files

1. *EtaNPV_Reactor_Optimization184B.m*
 - This code iterates through temperatures and pressures of interest, calling *EtAcetateReactor_PBR_Ideal_184B.m*. It ignores the separation system as that is only costed at discrete points. It then performs an economic analysis, costing all equipment, chemicals, and energy required to generate a series of cashflows which are then used to calculate the NPV of the project.
2. *Discrete_EtaNPV_Reactor_Optimization184B.m*
 - *This code operates on the same chasis that the former code does, except that it only calculates economic parameters at discrete points. These points line up for specific conversions at 240C and 2 atm only. These discrete points allow the code to include data about the separations system from Aspen plus models in order to compare the cost of separating reactor effluents at different conversions.*
3. *EtAcetateReactor_PBR_Ideal_184B.m*
 - This function calculates the plugged flow reactor conditions when called using an ODE solver, outputting molar flows at various volumes in the PFR.
4. *Sensitivity_HYSYS_EthylAcetate.m*
 - This function uses the base case parameters from the HYSYS flowsheet to calculate the NPV of the project as a function of various parameters such as chemical costs and tax rates. This function can be used for sensitivity analysis and is called by *MonteCarlo_TriangleDist_EthylAcetate.m*.
5. *MonteCarlo_TriangleDist_EthylAcetate.m*
 - This code performs a Monte Carlo simulation on the NPV of the project by assigning triangle distributions to each of the variables of interest, randomizing them N times, and calling *Sensitivity_HYSYS_EthylAcetate.m* to calculate the NPV. Then a probability distribution function and cumulative distribution function are created and plotted.

```
clear
close all
tic
%this script solves the concentration profiles in our isothermal ideal pfr
%neglecting pressure drop to determine the selectivities, toluene
%conversion, and molar flow streams for a desired production rate of
%ethyl acetate

%additionally this script determines revenue from flow streams from the
%separated components, and calculates NPV, TCI, ROI, and IRR from cash
%flows
Price.EtA = 1100;[$/MT]
Price.Ethanol = 500;[$/MT]
Price.Fuel = 2.5;[$/MM BTU]
Price.Electricity = 0.08; % $/kw hr
Price.CO2 = 40; %$/MT
Price.Cat = 10000; %$/MT
MW.EtA = 88.11;[g/gmol]
MW.Ethanol = 46.07;[g/gmol]
MW.Acetaldehyde = 44.05;[g/gmol]
MW.Ether = 74.12;[g/gmol]
MW.H2 = 2.02;[g/gmol]

lambda.EtA = 38.0; %kJ/mol, latent heat of evaporation
lambda.Ethanol = 42.3; %kJ/mol, latent heat of evaporation
lambda.Ether = 33.8; %kJ/mol, latent heat of evaporation

Cp.EthanolGas = 74/1000; %kJ/mol*K
Cp.EthanolLiq = 118/1000; %kJ/mol*K

dHcomb.H2 = 286; % kJ/mol

MethaneEnergy = 891; %kJ/gmol
MethaneCarbon = 1; %kJ/gmol

EnterpriseRate = 0.1;
ConstructionInterestRate = 0.05;
IncomeTaxRate = 0.27;
FCImultiplier = 1;
SUMultiplier = 1;
WCMultiplier = 1;

% P = 10; %[atm]
R = 0.08206; %[L*atm/K*mol]
R = R*1.01325; %[L*bar/K*mol]
F = 50;[gmol/hr] basis flowrate used to solve system before scale up
PEtA = 67556; [gmol/hr]
Vmax = 20; %[L]
labelT = {'T225' 'T230' 'T235' 'T240'};
labelP = {'P2' 'P4' 'P6' 'P8' 'P10'};
```

```

cc=length(length(labelP));
for j = 2:2:10
    P = j; %bar
    countP = (j-2)/2 + 1;
    for i = 225:5:240
        countT = (i - 225)/5 + 1;
        T = i + 273;
        %assume reactor feed is pure toluene and equal to plant feed stream of
        %toluene
        Q = [1 0 0 0 0 0]*F; %feed molar flowrate in gmol/hr
        %solve ode
        resolution = 500;
        Vspan = [0:(Vmax/resolution):Vmax];
        %       Vspan = logspace(-3,log10(Vmax),1001);
        opts = odeset('RelTol',1e-12,'AbsTol',1e-12);
        [Vout, Nout] = ode15s(@(V,N) EtAcetateReactor_PBR_Ideal_184B(V,N,T,P),Vspan,Q,
opts);
        %store output of ode45 in structures containing all values at different
        %temperatures
        V.(labelP{countP}).(labelT{countT}) = Vout(2:end);
        Ethanol.(labelP{countP}).(labelT{countT}) = Nout(2:end,1);
        Acetaldehyde.(labelP{countP}).(labelT{countT}) = Nout(2:end,2);
        H2.(labelP{countP}).(labelT{countT}) = Nout(2:end,3);
        EtA.(labelP{countP}).(labelT{countT}) = Nout(2:end,4);
        Ether.(labelP{countP}).(labelT{countT}) = Nout(2:end,5);
        H2O.(labelP{countP}).(labelT{countT}) = Nout(2:end,6);

        %compute tau for all reactor sizes output from ode45
        for new = 1:length(V.(labelP{countP}).(labelT{countT}))
            tau.(labelP{countP}).(labelT{countT})(new,1) = Vout(new)*P./(R*T*sum(Nout
(new,:)));
        end
        %calculate selectivity and conversion for selected T and Ft
        Ft = F;
        xt.(labelP{countP}).(labelT{countT}) = (Ft - Ethanol.(labelP{countP}).(labelT
{countT}))./Ft;%reactor conversion of Ethanol
        sEtA.(labelP{countP}).(labelT{countT}) = EtA.(labelP{countP}).(labelT
{countT})./((1/l)*(Ft - Ethanol.(labelP{countP}).(labelT{countT})));%reactor
selectivity for EtA
        sEther.(labelP{countP}).(labelT{countT}) = Ether.(labelP{countP}).(labelT
{countT})./((1/l)*(Ft - Ethanol.(labelP{countP}).(labelT{countT})));%reactor
selectivity for Ether

        %calculate real molar feeds, volumetric flow, and total reactor volume
        %at full scale
        FEthanol.(labelP{countP}).(labelT{countT}) = PEtA./(xt.(labelP{countP}).(labelT
{countT})).*sEtA.(labelP{countP}).(labelT{countT}));%feed reate of Ethanol to reactor
for desired PEtA [gmol/hr]
        qreal.(labelP{countP}).(labelT{countT}) = R*T*FEthanol.(labelP{countP}).(labelT
{countT})/P;%real volumetric flowrate [L/hr]

```

```

Vreal.(labelP{countP}).(labelT{countT}) = tau.(labelP{countP}).(labelT{
countT})*qreal.(labelP{countP}).(labelT{countT});%real reactor total volume [L]

%calculate the product molar flowrates from full scale reactor
PEther.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{
countT})*xt.(labelP{countP}).(labelT{countT})*sEther.(labelP{countP}).(labelT{
countT});%Product molar flow Ether [gmol/hr]
PH2O.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{
countT});
PEthanol.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{
countT})*(1-xt.(labelP{countP}).(labelT{countT}));%Product molar flow Ethanol
[gmol/hr]
PH2.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{
countT}) - PEthanol.(labelP{countP}).(labelT{countT});%Product molar flow Hydrogen
[gmol/hr]
PTotal.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{
countT})+PEthanol.(labelP{countP}).(labelT{countT})+PH2.(labelP{countP}).(labelT{
countT})+PH2O.(labelP{countP}).(labelT{countT})+PEtA;

%create vectors of mass flowrates
PMEther.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{
countT})*MW.Ether./(10^3);%[kg/hr]
PMEthanol.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{
countT})*MW.Ethanol./(10^3);%[kg/hr]
FMEthanol.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{
countT})*MW.Ethanol./(10^3);%[kg/hr]
PMEtA.(labelP{countP}).(labelT{countT}) = (PEtA*MW.EtA/(10^3)).*ones(length
(PEthanol.(labelP{countP}).(labelT{countT})),1);%[kg/hr]

%calculate the fresh feed stream flowrate assuming perfect separations
FreshFeed.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{
countT})-PEthanol.(labelP{countP}).(labelT{countT});
FreshFeedM.(labelP{countP}).(labelT{countT}) = FreshFeed.(labelP{countP}).(
labelT{countT})*MW.Ethanol./(10^3);%[kg/hr]

%%equipment costs
%reactor - sufficiently estimated with single tubular reactor cost
VR.(labelP{countP}).(labelT{countT}) = Vreal.(labelP{countP}).(labelT{countT})
/1000; %m^3
VR.(labelP{countP}).(labelT{countT}) = VR.(labelP{countP}).(labelT{countT})*
(3.28^3); %ft^3
Fm = 2.25; %stainless steel - H2 embrittlement
% pressure correction
if P < 3.45
    Fp = 1.00;
elseif P < 6.9
    Fp = 1.05;
elseif P < 13.8
    Fp = 1.15;
elseif P < 20.7

```

```

        Fp = 1.20;
elseif P < 27.6
    Fp = 1.35;
elseif P < 34.5
    Fp = 1.45;
end
Fc = Fm*Fp;
MS = 1650;
%set L:D ratio
D.(labelP{countP}).(labelT{countT}) = ((4/10)*(VR.(labelP{countP}).(labelT{countT}))/pi)).^(1/3); %ft
H.(labelP{countP}).(labelT{countT}) = 10*D.(labelP{countP}).(labelT{countT}); %ft
Area.(labelP{countP}).(labelT{countT}) = pi*(D.(labelP{countP}).(labelT{countT})).^2; %ft^2
ReactorCost.(labelP{countP}).(labelT{countT}) = (MS/280)*101.9*(D.(labelP{countP}).(labelT{countT}))^1.066.*(H.(labelP{countP}).(labelT{countT}))^0.82*(2.18+Fc);
ReactorCost.(labelP{countP}).(labelT{countT}) = ReactorCost.(labelP{countP}).(labelT{countT})/1e6; %MM$/yr

% feed furnace
eff = 0.70; % typical furnace efficiency
bp.Ethanol = 8*P+70; %linear approximation from phase diagram
Tf1 = 25;
Tf2 = bp.Ethanol;
T01 = bp.Ethanol;
T02 = T - 273;
QH2.(labelP{countP}).(labelT{countT}) = (eff)*PH2.(labelP{countP}).(labelT{countT})*dHcomb.H2; %kJ/hr
Qtotal.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT})*(lambda.Ethanol + ...
    (Tf2-Tf1)*Cp.EthanolLiq + (T02-T01)*Cp.EthanolGas); %kJ/hr
for c = 1:length(QH2.(labelP{countP}).(labelT{countT}))
    if QH2.(labelP{countP}).(labelT{countT})(c) > Qtotal.(labelP{countP}).(labelT{countT})(c)
        Qfurnace.(labelP{countP}).(labelT{countT})(c,1) = Qtotal.(labelP{countP}).(labelT{countT})(c);
        Qresid.(labelP{countP}).(labelT{countT})(c,1) = 0;
    elseif Qtotal.(labelP{countP}).(labelT{countT})(c) > QH2.(labelP{countP}).(labelT{countT})(c)
        Qfurnace.(labelP{countP}).(labelT{countT})(c,1) = QH2.(labelP{countP}).(labelT{countT})(c);
        Qresid.(labelP{countP}).(labelT{countT})(c,1) = Qtotal.(labelP{countP}).(labelT{countT})(c) - QH2.(labelP{countP}).(labelT{countT})(c);
    end
end
Qfurnace.(labelP{countP}).(labelT{countT}) = Qfurnace.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM BTU/hr

```



```

%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = H2carbon*PH2.✓
(labelP{countP}).(labelT{countT}); %gmol/hr
%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.✓
(labelP{countP}).(labelT{countT})*44.01/1000; %kg/hr
%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.✓
(labelP{countP}).(labelT{countT})*(24*50*7)/1000; %MT/year
FurnaceCarbon.(labelP{countP}).(labelT{countT}) = zeros(length(QH2.(labelP{countP}).(labelT{countT})),1); %no carbon production from H2 combustion
Fc = 1.5;
FurnaceCost.(labelP{countP}).(labelT{countT}) = (MS/280)*(5.07e3) ...
*(Qfurnace.(labelP{countP}).(labelT{countT}).^0.85)*(1.23+Fc); %$
FurnaceCost.(labelP{countP}).(labelT{countT}) = FurnaceCost.(labelP{countP}).(labelT{countT})/1e6; %MM$

% feed heat exchangers
SteamTemp = 139; %50psig sat steam

for c = 1:length(QH2.(labelP{countP}).(labelT{countT}))
    if QH2.(labelP{countP}).(labelT{countT})(c) > Qtotal.(labelP{countP}).(labelT{countT})(c)
        %heat exchanger 1:
        T01 = 25; %C
        Tf1(c,1) = Qresid.(labelP{countP}).(labelT{countT})(c)./(FEthanol.✓
(labelP{countP}).(labelT{countT})(c).*Cp.EthanolLiq);
        dTA = SteamTemp - T01; %inlet temp difference
        dTB(c,1) = SteamTemp - Tf1(c); %outlet temp difference
        %sensible heat
        FeedHeating.(labelP{countP}).(labelT{countT})(c,1) = Qresid.(labelP{countP}).(labelT{countT})(c); %kJ/hr
        FeedHeatinghr.(labelP{countP}).(labelT{countT})(c,1) = FeedHeating.✓
(labelP{countP}).(labelT{countT})(c)*0.947817/1e6; %MM Btu/hr
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = FeedHeatinghr.✓
(labelP{countP}).(labelT{countT})(c)*Price.Fuel*0.7; %$/hr (from table E.1-1)
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = H1SteamCost.✓
(labelP{countP}).(labelT{countT})(c)*(24*7*50)/1e6; %MM$/yr
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = 0; %MM$/yr %✓
    assume heat integration with feed effluent
        % will be ingnored as design includes HX integration
        dTlm(c,1) = (dTA - dTB(c))./(log(dTA./dTB(c))); %approximation for log✓
    mean temp diff
        dTlm(c,1) = dTlm(c)*9/5 + 32; %F
        elseif Qtotal.(labelP{countP}).(labelT{countT})(c) > QH2.(labelP{countP}).(labelT{countT})(c)
            dTlm(c,1) = 1;
            FeedHeatinghr.(labelP{countP}).(labelT{countT})(c,1) = 0;
            H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = 0; %MM$/yr %✓
        assume heat integration with feed effluent
    end
end
end

```

```

U = 150; %BTU/ft^2 F h
eta = 0.7;
A = (eta)*FeedHeatinghr.(labelP{countP}).(labelT{countT})*1e6./(U.*dTlm); %ft^2
Fm = 2.81; %material correction, stainless steel
Fd = 1; %design correction
if P < 20.7
    Fp = 0; %pressure correction
elseif P < 27.6
    Fp = 0.1;
elseif P < 55.2
    Fp = 0.25;
end
Fc = (Fd + Fp)*Fm;
HXlQ.(labelP{countP}).(labelT{countT}) = FeedHeating.(labelP{countP}).(labelT{countT}); %kJ/hr
HXcost1.(labelP{countP}).(labelT{countT}) = (MS/280)*101.3*(A.^0.65)*(2.29+Fc); %$

HXcost.(labelP{countP}).(labelT{countT}) = HXcost1.(labelP{countP}).(labelT{countT})/1e6; %MM$

HeatOPCost.(labelP{countP}).(labelT{countT}) = HlSteamCost.(labelP{countP}).(labelT{countT}); %MM$ /yr

%%separation system
PSepTotal.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{countT})+PH2O.(labelP{countP}).(labelT{countT})+PEtA;
XH2O.(labelP{countP}).(labelT{countT}) = PH2O.(labelP{countP}).(labelT{countT})./PSepTotal.(labelP{countP}).(labelT{countT});
XEthanol.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{countT})./PSepTotal.(labelP{countP}).(labelT{countT});
XEtA.(labelP{countP}).(labelT{countT}) = PEtA./PSepTotal.(labelP{countP}).(labelT{countT});

for y = 1
    % distillation column 1
    % Dist1P = 1; %bar
    % Dist1T = 100; %C
    % aa = 12.5;
    % ab = 4.5;
    % ac = 2.1;
    % ad = 1;
    % aij = 2.33;
    % xa = PEther.(labelP{countP}).(labelT{countT})./PTotal.(labelP{countP}).(labelT{countT});
    % xb = PEthanol.(labelP{countP}).(labelT{countT})./PTotal.(labelP{countP}).(labelT{countT});
    % xc = PEtA./PTotal.(labelP{countP}).(labelT{countT});
    % xd = PEther.(labelP{countP}).(labelT{countT})./PTotal.(labelP{countP}).(labelT{countT});

```

```

%          Dist1MvFeed = xa.*MW.Ether + xb.*MW.Ethanol + xc.*MW.EtA + xd.✓
*MW.Ether;
%          Dist1MvDist = xa.*MW.Ether./xa;
%          Dist1MvBottoms = (xb.*MW.Ethanol + xc.*MW.EtA + xd.*MW.Ether).*(✓
(1./(xb+xc+xd)));
%          splitttype = 4;
%          Dist1rmin = rminCalc(aa,ab,ac,ad,xa,xb,xc,xd,splitttype); %table✓
4.1 revised
%          Dist1lambdaD = lambda.Benzene; %latent heat of distillate mixture
%          Dist1lambdaB = (xb.*lambda.Tol + xc.*lambda.ParaX + xd.*lambda.✓
TMB).*(1./(xb+xc+xd)); %latent heat of bottoms mixture
%          Dist1F = PEther.(labelP{countP}).(labelT{countT}) + PEthanol.✓
(labelP{countP}).(labelT{countT}) ...
%          + PEther.(labelP{countP}).(labelT{countT}) + PEtA;
%          Dist1zF = xa;
%          [Dist1Qc.(labelP{countP}).(labelT{countT}),Dist1Qr.(labelP{✓
{countP}).(labelT{countT}),...
%          Dist1H.(labelP{countP}).(labelT{countT}),Dist1D.(labelP{✓
{countP}).(labelT{countT}), ...
%          Dist1Nreal.(labelP{countP}).(labelT{countT}),Dist1r.(labelP{✓
{countP}).(labelT{countT}),...
%          Dist1s.(labelP{countP}).(labelT{countT}),Dist1VoverF.(labelP{✓
{countP}).(labelT{countT})]...
%          = dist_column(Dist1F,Dist1zF,Dist1rmin,Dist1P,Dist1T,✓
Dist1lambdaD,Dist1lambdaB,Dist1MvFeed,Dist1MvDist,Dist1MvBottoms,aij);
%          Dist1DSattemp = 80.1; %deg C, BP of benzene
%          Dist1BSattemp = 110; %deg C, BP of bottoms mixture, estimate
%          Dist1CoolingWaterCoolTemp = 25; % deg C
%          Dist1CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg✓
C
%          Dist1SteamTemp = 194; % deg C, 200 psia steam
%          Dist1dTlmD.(labelP{countP}).(labelT{countT}) = ...
%          ((Dist1DSattemp - Dist1CoolingWaterCoolTemp) - (Dist1DSattemp✓
- Dist1CoolingWaterHotTemp))/...
%          log((Dist1DSattemp - Dist1CoolingWaterCoolTemp)/✓
(Dist1DSattemp - Dist1CoolingWaterHotTemp));
%          Dist1dTlmB.(labelP{countP}).(labelT{countT}) = (Dist1SteamTemp -✓
Dist1BSattemp);
%          Dist1UD = 770; %W/m^2 K
%          Dist1UD = Dist1UD*60*60/1000; %kJ/hr m^2 K
%          Dist1UB = 820; %W/m^2 K
%          Dist1UB = Dist1UB*60*60/1000; %kJ/hr m^2 K
%          Dist1AreaD.(labelP{countP}).(labelT{countT}) = Dist1Qc.(labelP{✓
{countP}).(labelT{countT})./(Dist1UD.*Dist1dTlmD.(labelP{countP}).(labelT{countT})); %✓
m^2
%          Dist1AreaB.(labelP{countP}).(labelT{countT}) = Dist1Qr.(labelP{✓
{countP}).(labelT{countT})./(Dist1UB.*Dist1dTlmB.(labelP{countP}).(labelT{countT})); %✓
m^2
%
%          Fd = 1;

```

```

%      P0 = 11; %bar
%      Fp = 0.10*(Dist1P-P0)./P0;
%      Fm = 1;
%      Fi = 1.38;
%      FD = 2.3;
%      ah = 0.65;
%      A0 = 93; %m^2
%      Dist1HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist1AreaD.(labelP{
countP}).(labelT{countT})./A0).^ah);
%      Dist1HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist1AreaB.(labelP{
countP}).(labelT{countT})./A0).^ah);
%
%      Fm = 1;
%      P0 = 4.5; %bar
%      t_p = 0.13*(Dist1P-P0)./P0;
%      Fp = 1+t_p*(1+exp(-t_p./2));
%      Fi = 1.38;
%      Fd = 3;
%      Fs = 1; % (for 60 cm tray spacing)
%      Ft = 0; %sieve
%      d.(labelP{countP}).(labelT{countT}) = Dist1D.(labelP{countP}).
(labelT{countT});
%      d0 = 1; %m
%      H0 = 6.1; %m
%      as = 0.82;
%      at = 1.8;
%      CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(d.(labelP{
countP}).(labelT{countT})./d0).*((Dist1H.(labelP{countP}).(labelT{countT})./H0).^as); %$
%
%      CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*((d.(labelP{countP}).
(labelT{countT})./d0).^at).*(Dist1H.(labelP{countP}).(labelT{countT})./H0); %$
%      Dist1ColumnCost.(labelP{countP}).(labelT{countT}) = (CostShell +
CostTray)/10; %$
%
%      Dist1QcBTU.(labelP{countP}).(labelT{countT}) = Dist1Qc.(labelP{
countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
%      Dist1HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist1QcBTU.
(labelP{countP}).(labelT{countT})*Price.Fuel*1.13; %$/hr
%      Dist1HXDOpCost.(labelP{countP}).(labelT{countT}) =
Dist1HXDOpCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%
%      Dist1QrBTU.(labelP{countP}).(labelT{countT}) = Dist1Qr.(labelP{
countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
%      Dist1HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist1QrBTU.
(labelP{countP}).(labelT{countT})*Price.Fuel*0.93; %$/hr
%      Dist1HXBOPCost.(labelP{countP}).(labelT{countT}) =
Dist1HXBOPCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%

```

```

%           %distillation column 2
%           Dist2P = 1; %bar
%           Dist2T = 100; %C
%           aa = 4.5;
%           ab = 2.1;
%           ac = 1;
%           ad = 1;
%           aij = 2.2;
%           xa = PEthanol.(labelP{countP}).(labelT{countT})./(PTotal.(labelP{countP}).(labelT{countT})-PEther.(labelP{countP}).(labelT{countT}));
%           xb = PEtA./(PTotal.(labelP{countP}).(labelT{countT})-PEther.(labelP{countP}).(labelT{countT}));
%           xc = PEther.(labelP{countP}).(labelT{countT})./(PTotal.(labelP{countP}).(labelT{countT})-PEther.(labelP{countP}).(labelT{countT}));
%           xd = 0;
%           Dist2MvFeed = xa.*MW.Ethanol + xb.*MW.EtA + xc.*MW.Ether;
%           Dist2MvDist = xa.*MW.Ethanol./xa;
%           Dist2MvBottoms = (xb.*MW.EtA + xc.*MW.Ether).*(1./(xb+xc));
%           splitttype = 1;
%           Dist2rmin = rminCalc(aa,ab,ac,ad,xa,xb,xc,xd,splitttype); %table
4.1 revised
%           Dist2lambdaD = lambda.Tol; %latent heat of distillate mixture
%           Dist2lambdaB = (xb.*lambda.ParaX + xc.*lambda.TMB).*(1./(xb+xc));
%latent heat of bottoms mixture
%           Dist2F = PEthanol.(labelP{countP}).(labelT{countT}) + PEther.(labelP{countP}).(labelT{countT}) + PEtA;
%           Dist2zF = xa;
%           [Dist2Qc.(labelP{countP}).(labelT{countT}),Dist2Qr.(labelP{countP}).(labelT{countT}),...
%           Dist2H.(labelP{countP}).(labelT{countT}),Dist2D.(labelP{countP}).(labelT{countT}), ...
%           Dist2Nreal.(labelP{countP}).(labelT{countT}),Dist2r.(labelP{countP}).(labelT{countT}),...
%           Dist2s.(labelP{countP}).(labelT{countT}),Dist2VoverF.(labelP{countP}).(labelT{countT})]...
%           = dist_column(Dist2F,Dist2zF,Dist2rmin,Dist2P,Dist2T,
Dist2lambdaD,Dist2lambdaB,Dist2MvFeed,Dist2MvDist,Dist2MvBottoms,aij);
%           Dist2DSattemp = 111; %deg C, BP of toluene
%           Dist2BSattemp = 125; %deg C, BP of bottoms mixture, estimate
%           Dist2CoolingWaterCoolTemp = 25; % deg C
%           Dist2CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg
C
%           Dist2SteamTemp = 194; % deg C, 200 psia steam
%           Dist2dTlmD.(labelP{countP}).(labelT{countT}) = ...
%           ((Dist2DSattemp - Dist2CoolingWaterCoolTemp) - (Dist2DSattemp
- Dist2CoolingWaterHotTemp))/...
%           log((Dist2DSattemp - Dist2CoolingWaterCoolTemp)/
(Dist2DSattemp - Dist2CoolingWaterHotTemp));
%           Dist2dTlmB.(labelP{countP}).(labelT{countT}) = (Dist2SteamTemp -
Dist2BSattemp);

```

```

%      Dist2UD = 770; %W/m^2 K
%      Dist2UD = Dist2UD*60*60/1000; %kJ/hr m^2 K
%      Dist2UB = 820; %W/m^2 K
%      Dist2UB = Dist2UB*60*60/1000; %kJ/hr m^2 K
%      Dist2AreaD.(labelP{countP}).(labelT{countT}) = Dist2Qc.(labelP{countP}).(labelT{countT})./(Dist2UD.*Dist2dTlmD.(labelP{countP}).(labelT{countT})); %m^2
%      Dist2AreaB.(labelP{countP}).(labelT{countT}) = Dist2Qr.(labelP{countP}).(labelT{countT})./(Dist2UB.*Dist2dTlmB.(labelP{countP}).(labelT{countT})); %m^2
%
%      Fd = 1;
%      P0 = 11; %bar
%      Fp = 0.10*(Dist2P-P0)./P0;
%      Fm = 1;
%      Fi = 1.38;
%      FD = 2.3;
%      ah = 0.65;
%      A0 = 93; %m^2
%      Dist2HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
%      (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist2AreaD.(labelP{countP}).(labelT{countT}))./A0).^ah);
%      Dist2HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
%      (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist2AreaB.(labelP{countP}).(labelT{countT}))./A0).^ah);
%
%      Fm = 1;
%      P0 = 4.5; %bar
%      t_p = 0.13*(Dist2P-P0)./P0;
%      Fp = 1+t_p*(1+exp(-t_p./2));
%      Fi = 1.38;
%      Fd = 3;
%      Fs = 1; % (for 60 cm tray spacing)
%      Ft = 0; %sieve
%      d.(labelP{countP}).(labelT{countT}) = Dist2D.(labelP{countP}).(labelT{countT});
%      d0 = 1; %m
%      H0 = 6.1; %m
%      as = 0.82;
%      at = 1.8;
%      CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(d.(labelP{countP}).(labelT{countT}))./d0).*((Dist2H.(labelP{countP}).(labelT{countT}))./H0).^as); %$
%
%      CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*((d.(labelP{countP}).(labelT{countT}))./d0).^at).*(Dist2H.(labelP{countP}).(labelT{countT}))./H0); %$
%      Dist2ColumnCost.(labelP{countP}).(labelT{countT}) = (CostShell + CostTray)/10; %$
%
%      Dist2QcBTU.(labelP{countP}).(labelT{countT}) = Dist2Qc.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr

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%          Dist2HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist2QcBTU.✓
(labelP{countP}).(labelT{countT})*Price.Fuel*1.13; %$/hr
%          Dist2HXDOpCost.(labelP{countP}).(labelT{countT}) =✓
Dist2HXDOpCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%
%          Dist2QrBTU.(labelP{countP}).(labelT{countT}) = Dist2Qr.(labelP✓
{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
%          Dist2HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist2QrBTU.✓
(labelP{countP}).(labelT{countT})*Price.Fuel*0.93; %$/hr
%          Dist2HXBOPCost.(labelP{countP}).(labelT{countT}) =✓
Dist2HXBOPCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%
%          %distillation column 3
%          Dist3P = 1; %bar
%          Dist3T = 100; %C
%          aa = 2.1;
%          ab = 1;
%          ac = 1;
%          ad = 1;
%          aij = 2.1;
%          xa = PEtA./(PEtA+PEther.(labelP{countP}).(labelT{countT}));
%          xb = PEther.(labelP{countP}).(labelT{countT})./(PEtA+PEther.✓
(labelP{countP}).(labelT{countT}));
%          xc = 0;
%          xd = 0;
%          MvFeed = xa.*MW.EtA + xb.*MW.Ether;
%          MvDist = xa.*MW.EtA./xa;
%          MvBottoms = xb.*MW.Ether./xb;
%          splittype = 10;
%          Dist3rmin = rminCalc(aa,ab,ac,ad,xa,xb,xc,xd,splittype); %table✓
4.1 revised
%          Dist3lambdaD = lambda.ParaX; %latent heat of distillate mixture
%          Dist3lambdaB = lambda.TMB; %latent heat of bottoms mixture
%          Dist3F = PEther.(labelP{countP}).(labelT{countT}) + PEtA;
%          Dist3zF = xa;
%          [Dist3Qc.(labelP{countP}).(labelT{countT}),Dist3Qr.(labelP✓
{countP}).(labelT{countT}),...
%          Dist3H.(labelP{countP}).(labelT{countT}),Dist3D.(labelP✓
{countP}).(labelT{countT}), ...
%          Dist3Nreal.(labelP{countP}).(labelT{countT}),Dist3r.(labelP✓
{countP}).(labelT{countT}),...
%          Dist3s.(labelP{countP}).(labelT{countT}),Dist3VoverF.(labelP✓
{countP}).(labelT{countT})]...
%          = dist_column(Dist3F,Dist3zF,Dist3rmin,Dist3P,Dist3T,✓
Dist3lambdaD,Dist3lambdaB,MvFeed,MvDist,MvBottoms,aij);
%          Dist3DSattemp = 138.4; %deg C, BP of paraX
%          Dist3BSattemp = 170; %deg C, BP of bottoms mixture, estimate
%          Dist3CoolingWaterCoolTemp = 25; % deg C
%          Dist3CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg✓

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%          Dist3SteamTemp = 250; % deg C, 600 psia steam
%          Dist1dTlmD.(labelP{countP}).(labelT{countT}) = ...
%          ((Dist3DSattemp - Dist3CoolingWaterCoolTemp) - (Dist3DSattemp
- Dist3CoolingWaterHotTemp))/...
%          log((Dist3DSattemp - Dist3CoolingWaterCoolTemp)/
(Dist3DSattemp - Dist3CoolingWaterHotTemp));
%          Dist3dTlmB.(labelP{countP}).(labelT{countT}) = (Dist3SteamTemp -
Dist3BSattemp);
%          Dist3UD = 770; %W/m^2 K
%          Dist3UD = Dist3UD*60*60/1000; %kJ/hr m^2 K
%          Dist3UB = 820; %W/m^2 K
%          Dist3UB = Dist3UB*60*60/1000; %kJ/hr m^2 K
%          Dist3AreaD.(labelP{countP}).(labelT{countT}) = Dist3Qc.(labelP
{countP}).(labelT{countT})./(Dist3UD.*Dist2dTlmD.(labelP{countP}).(labelT{countT})); %
m^2
%          Dist3AreaB.(labelP{countP}).(labelT{countT}) = Dist3Qr.(labelP
{countP}).(labelT{countT})./(Dist3UB.*Dist2dTlmB.(labelP{countP}).(labelT{countT})); %
m^2
%
%          Fd = 1;
%          P0 = 11; %bar
%          Fp = 0.10*(Dist3P-P0)./P0;
%          Fm = 1;
%          Fi = 1.38;
%          FD = 2.3;
%          ah = 0.65;
%          A0 = 93; %m^2
%          Dist3HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301)*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist3AreaD.(labelP
{countP}).(labelT{countT})./A0).^ah);
%          Dist3HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301)*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist3AreaB.(labelP
{countP}).(labelT{countT})./A0).^ah);
%
%          Fm = 1;
%          P0 = 4.5; %bar
%          t_p = 0.13*(Dist3P-P0)./P0;
%          Fp = 1+t_p*(1+exp(-t_p./2));
%          Fi = 1.38;
%          Fd = 3;
%          Fs = 1; % (for 60 cm tray spacing)
%          Ft = 0; %sieve
%          d.(labelP{countP}).(labelT{countT}) = Dist3D.(labelP{countP}).
(labelT{countT});
%          d0 = 1; %m
%          H0 = 6.1; %m
%          as = 0.82;
%          at = 1.8;
%          CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(d.(labelP
{countP}).(labelT{countT})./d0).*((Dist3H.(labelP{countP}).(labelT{countT})./H0).^as);

```



```

%$
%           CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*((d.(labelP{countP})).✓
(labelT{countT})./d0).^at).*(Dist3H.(labelP{countP})).(labelT{countT})./H0); %$
%           Dist3ColumnCost.(labelP{countP})).(labelT{countT})) = (CostShell +✓
CostTray)/10; %$
%
%           Dist3QcBTU.(labelP{countP})).(labelT{countT})) = Dist3Qc.(labelP✓
{countP})).(labelT{countT}))*0.947817/1e6; %MM Btu/hr
%           Dist3HXDOpCost.(labelP{countP})).(labelT{countT})) = Dist3QcBTU.✓
(labelP{countP})).(labelT{countT}))*Price.Fuel*1.13; %$/hr
%           Dist3HXDOpCost.(labelP{countP})).(labelT{countT})) =✓
Dist3HXDOpCost.(labelP{countP})).(labelT{countT}))* (24*7*50)/1e6; %MM$/yr
%
%           Dist3QrBTU.(labelP{countP})).(labelT{countT})) = Dist3Qr.(labelP✓
{countP})).(labelT{countT}))*0.947817/1e6; %MM Btu/hr
%           Dist3HXBOPCost.(labelP{countP})).(labelT{countT})) = Dist3QrBTU.✓
(labelP{countP})).(labelT{countT}))*Price.Fuel*1.13; %$/hr
%           Dist3HXBOPCost.(labelP{countP})).(labelT{countT})) =✓
Dist3HXBOPCost.(labelP{countP})).(labelT{countT}))* (24*7*50)/1e6; %MM$/yr
%
%
%           %Sum of all three columns
%           DistSteamEnergy.(labelP{countP})).(labelT{countT})) = ... %kJ/hr
%           Dist1Qr.(labelP{countP})).(labelT{countT})) + ...
%           Dist2Qr.(labelP{countP})).(labelT{countT})) + ...
%           Dist3Qr.(labelP{countP})).(labelT{countT}));
%           DistCost.(labelP{countP})).(labelT{countT})) = ... $
%           Dist1HXDCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist1HXBCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist2HXDCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist2HXBCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist3HXDCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist3HXBCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist1ColumnCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist2ColumnCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist3ColumnCost.(labelP{countP})).(labelT{countT}));
%           DistCost.(labelP{countP})).(labelT{countT})) = DistCost.(labelP✓
{countP})).(labelT{countT}))/1e6; %MM$
%           DistOpCost.(labelP{countP})).(labelT{countT})) = ...
%           Dist1HXDOpCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist2HXDOpCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist3HXDOpCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist1HXBOPCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist2HXBOPCost.(labelP{countP})).(labelT{countT})) + ...
%           Dist3HXBOPCost.(labelP{countP})).(labelT{countT}));
end

DistCost.(labelP{countP})).(labelT{countT})) = zeros(length(A),1); %ignoring cost
%           DistCost.(labelP{countP})).(labelT{countT})) = 2.5./xt.(labelP✓
{countP})).(labelT{countT})); %MM$ %using fake correlation

```

```

        DistOpCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring
operating cost
        %           DistOpCost.(labelP{countP}).(labelT{countT}) = (500000./xt.(labelP
{countP}).(labelT{countT}))/1e6; %MM$ %using fake correlation
        DistSteamEnergy.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %
ignoring cost %kJ/hr

        %turbine
        gamma = 0.23;
        Pin = 1*2116.22; %lbf/ft^2
        Pout = P*2116.22; %lbf/ft^2
        Qin = (1/60)*0.0353147.*PTotal.(labelP{countP}).(labelT{countT})*R*300/1; %
ft^3/min
        hp = (3.03e-5/gamma)*Pin.*Qin*((Pout/Pin)^gamma - 1);
        bhp = hp/0.8;
        Fd = 1.15; %reciprocal, turbine
        Fc = Fd;
        TurbCost.(labelP{countP}).(labelT{countT}) = (MS/280)*517.5*(bhp.^0.82)*(2.11 +
Fc);
        TurbCost.(labelP{countP}).(labelT{countT}) = TurbCost.(labelP{countP}).(labelT
{countT}))/1e6;
        TurbCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
        %turbine operating costs
        TurbOPCost.(labelP{countP}).(labelT{countT}) = -(bhp/0.9)*(1/1.341)*Price.
Electricity*8400/1e6; % MM$/year
        TurbOPCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring
operating cost due to gained electricity powering pumps

        %carbon operating costs
        ElectricityCarbon.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
        SteamEnergy.(labelP{countP}).(labelT{countT}) = HX1Q.(labelP{countP}).(labelT
{countT}) + DistSteamEnergy.(labelP{countP}).(labelT{countT}); %kJ/hr
        FlowMethaneForSteam.(labelP{countP}).(labelT{countT}) = SteamEnergy.(labelP
{countP}).(labelT{countT})/MethaneEnergy; %gmol/hr
        SteamCarbon.(labelP{countP}).(labelT{countT}) =
MethaneCarbon*FlowMethaneForSteam.(labelP{countP}).(labelT{countT}); %gmol/hr
        SteamCarbon.(labelP{countP}).(labelT{countT}) = SteamCarbon.(labelP{countP}).
(labelT{countT})*44.01/1000; %kg/hr
        SteamCarbon.(labelP{countP}).(labelT{countT}) = SteamCarbon.(labelP{countP}).
(labelT{countT})*(24*50*7)/1000; %MT/year
        Carbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.(labelP{countP}).
(labelT{countT}) + ...
        ElectricityCarbon.(labelP{countP}).(labelT{countT}) + ...
        SteamCarbon.(labelP{countP}).(labelT{countT}); %including carbon costs, $
        CarbonCost.(labelP{countP}).(labelT{countT}) = Carbon.(labelP{countP}).(labelT
{countT})*Price.CO2/1e6; %MM$
        %           CarbonCost.(label{count}) = zeros(length(A),1); %ignoring carbon
costs

        % total upfront equipment costs

```

```

Equip.(labelP{countP}).(labelT{countT}) = HXcost.(labelP{countP}).(labelT{countT}) + ...
ReactorCost.(labelP{countP}).(labelT{countT}) + DistCost.(labelP{countP}).(labelT{countT}) + ...
TurbCost.(labelP{countP}).(labelT{countT}) + FurnaceCost.(labelP{countP}).(labelT{countT}); %MM$
FCI.(labelP{countP}).(labelT{countT}) = 2.28*Equip.(labelP{countP}).(labelT{countT}); %MM$
FCI.(labelP{countP}).(labelT{countT}) = FCImultiplier*FCI.(labelP{countP}).(labelT{countT}); %MM$ (for sensitivityanalysis)
SU.(labelP{countP}).(labelT{countT}) = 0.1*FCI.(labelP{countP}).(labelT{countT}); %MM$
SU.(labelP{countP}).(labelT{countT}) = SUMultiplier*SU.(labelP{countP}).(labelT{countT}); %MM$ (for sensitivityanalysis)
WC.(labelP{countP}).(labelT{countT}) = 2/12*FreshFeedM.(labelP{countP}).(labelT{countT})*Price.Ethanol/1000*24*7*50/1e6; %MM$/year
WC.(labelP{countP}).(labelT{countT}) = WCMultiplier*WC.(labelP{countP}).(labelT{countT}); %MM$ (for sensitivityanalysis)
TI.(labelP{countP}).(labelT{countT}) = FCI.(labelP{countP}).(labelT{countT}) + SU.(labelP{countP}).(labelT{countT}) + WC.(labelP{countP}).(labelT{countT}); %MM$

%loan amount
loan.(labelP{countP}).(labelT{countT}) = TI.(labelP{countP}).(labelT{countT});
%construction rate for first 2 years, 2% higher than corporate rate
ConstructionInterest.(labelP{countP}).(labelT{countT}) = loan.(labelP{countP}).(labelT{countT})*(ConstructionInterestRate);

%corporate bond cash flows, 3% (DOW/BASF), total amount of construction
%costs and interest up to that point, 10 year bond life (simple
%interest)
bond.(labelP{countP}).(labelT{countT}) = loan.(labelP{countP}).(labelT{countT}) + ConstructionInterest.(labelP{countP}).(labelT{countT}) + ...
ConstructionInterest.(labelP{countP}).(labelT{countT})*(1.05);
CorporateInterest.(labelP{countP}).(labelT{countT}) = bond.(labelP{countP}).(labelT{countT})*(0.03);

%chemical revenue, operating costs, and total revenuebefore taxes
Revenue.(labelP{countP}).(labelT{countT}) = (24*7*50)*(PMEtA.(labelP{countP}).(labelT{countT}))*Price.EtA + ...
PMEthanol.(labelP{countP}).(labelT{countT})*Price.Ethanol - FMEthanol.(labelP{countP}).(labelT{countT})*Price.Ethanol/(1e9); %MM$/yr
RevenueProducts.(labelP{countP}).(labelT{countT}) = (24*7*50)*(PMEtA.(labelP{countP}).(labelT{countT}))*Price.EtA/1e9; %MM$/yr
AGS.(labelP{countP}).(labelT{countT}) = 0.1*RevenueProducts.(labelP{countP}).(labelT{countT});
OperateCost.(labelP{countP}).(labelT{countT}) = DistOpCost.(labelP{countP}).(labelT{countT}) + ...
HeatOPCost.(labelP{countP}).(labelT{countT}) + TurbOPCost.(labelP{countP}).(labelT{countT}) + ...
CarbonCost.(labelP{countP}).(labelT{countT});

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```

% cost of manufacturing
COM.(labelP{countP}).(labelT{countT}) = OperateCost.(labelP{countP}).(labelT{countT}) + AGS.(labelP{countP}).(labelT{countT});

%salvage value, assuming 1% of initial equipment costs
salvage.(labelP{countP}).(labelT{countT}) = Equip.(labelP{countP}).(labelT{countT})*0.01/2;

%depreciation, linear over 10 years
deprec.(labelP{countP}).(labelT{countT}) = (FCI.(labelP{countP}).(labelT{countT}) + SU.(labelP{countP}).(labelT{countT}) ...
    - salvage.(labelP{countP}).(labelT{countT}))./10; %/year
tax = IncomeTaxRate;

%%calculate cash flows
%assign initial cash flows, assuming 60/40 split during construction
cashflow.year1.(labelP{countP}).(labelT{countT}) = zeros(length(A),1) + loan.
(labelP{countP}).(labelT{countT}); %land
cashflow.year2.(labelP{countP}).(labelT{countT}) = -(0.6)*FCI.(labelP{countP}).
(labelT{countT});
%startup capital
cashflow.year3.(labelP{countP}).(labelT{countT}) = -(0.4)*FCI.(labelP{countP}).
(labelT{countT}) - SU.(labelP{countP}).(labelT{countT}) - ...
    WC.(labelP{countP}).(labelT{countT}) - ConstructionInterest.(labelP{countP}).(labelT{countT});
%cashflows during 10 year depreciation and corporate bond period
for year = 4:12
    yearlist = ['year' num2str(year)];
    profit.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP{countP}).(labelT{countT}) - ...
        COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP{countP}).(labelT{countT}) - ...
        deprec.(labelP{countP}).(labelT{countT}));
    cashflow.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP{countP}).(labelT{countT}) - ...
        COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP{countP}).(labelT{countT}) - ...
        deprec.(labelP{countP}).(labelT{countT})).*(1-tax) + ...
        deprec.(labelP{countP}).(labelT{countT});
end
cashflow.year13.(labelP{countP}).(labelT{countT}) = Revenue.(labelP{countP}).
(labelT{countT}) - ...
    COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP{countP}).
(labelT{countT}) - ...
    loan.(labelP{countP}).(labelT{countT});
%after depreciation and bond life
for year = 14:18
    yearlist = ['year' num2str(year)];
    cashflow.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP{countP}).
(labelT{countT}) - ...

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        COM.(labelP{countP}).(labelT{countT})).*(1-tax);
    end
    % Before tax cash flows
    for year = 4:13
        yearlist = ['year' num2str(year)];
        cashflowBT.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP{countP}).(labelT{countT}) - ...
        COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP{countP}).(labelT{countT}));
    end
    for year = 14:18
        yearlist = ['year' num2str(year)];
        cashflowBT.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP{countP}).(labelT{countT}) - ...
        COM.(labelP{countP}).(labelT{countT}));
    end

    %salvage costs
    cashflow.year18.(labelP{countP}).(labelT{countT}) = cashflow.year18.(labelP{countP}).(labelT{countT}) + ...
    salvage.(labelP{countP}).(labelT{countT}) + WC.(labelP{countP}).(labelT{countT});

    %catalyst costs every 2 years
    CatalystVol.(labelP{countP}).(labelT{countT}) = Vreal.(labelP{countP}).(labelT{countT})*1000; %mL
    CatalystMass.(labelP{countP}).(labelT{countT}) = CatalystVol.(labelP{countP}).(labelT{countT})*0.5*6.31/1e6; %MT
    CatalystCost.(labelP{countP}).(labelT{countT}) = CatalystMass.(labelP{countP}).(labelT{countT})*Price.Cat/1e6; %MM$
    for year = 3:1:18
        yearlist = ['year' num2str(year)];
        cashflow.(yearlist).(labelP{countP}).(labelT{countT}) = cashflow.(yearlist).(labelP{countP}).(labelT{countT}) - ...
        CatalystCost.(labelP{countP}).(labelT{countT})*2;
    end
    cashflownoloans = cashflow;
    cashflownoloans.year1.(labelP{countP}).(labelT{countT}) = cashflownoloans.year1.(labelP{countP}).(labelT{countT}) - loan.(labelP{countP}).(labelT{countT});
    cashflownoloans.year13.(labelP{countP}).(labelT{countT}) = cashflownoloans.year13.(labelP{countP}).(labelT{countT}) + loan.(labelP{countP}).(labelT{countT});
    %%NPV calculation
    NPV.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
    for year = 1:18
        yearlist = ['year' num2str(year)];
        discount.(yearlist) = (1/((1+EnterpriseRate)^year));
        NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT}) = cashflow.(yearlist).(labelP{countP}).(labelT{countT})*discount.(yearlist);
        NPVcashflownoloan.(yearlist).(labelP{countP}).(labelT{countT}) = cashflownoloans.(yearlist).(labelP{countP}).(labelT{countT})*discount.(yearlist);
        NPV.(labelP{countP}).(labelT{countT}) = NPV.(labelP{countP}).(labelT{countT}) + NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT}) - NPVcashflownoloan.(yearlist).(labelP{countP}).(labelT{countT});
    end
end

```

```

(countT)) + NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT});
    end
    % cumulative cash flows
    CumulativeDiscountedCashFlowLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeDiscountedCashFlowNoLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeNonDiscountedCashFlowLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeNonDiscountedCashFlowNoLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);

    for year = 1:18
        yearlist = ['year' num2str(year)];
        yearlistprevious = ['year' num2str(year-1)];
        CumulativeDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{
(countT)) = ...
            CumulativeDiscountedCashFlowLoan.(yearlistprevious).(labelP{countP}).✓
(labelT{countT}) ...
            + NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{
(countT)) = ...
            CumulativeDiscountedCashFlowNoLoan.(yearlistprevious).(labelP{countP}).✓
(labelT{countT}) ...
            + NPVcashflownoloan.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeNonDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{
(countT)) = ...
            CumulativeNonDiscountedCashFlowLoan.(yearlistprevious).(labelP{
(countP)).(labelT{countT}) ...
            + cashflow.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeNonDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{
(countT)) = ...
            CumulativeNonDiscountedCashFlowLoan.(yearlistprevious).(labelP{
(countP)).(labelT{countT}) ...
            + cashflownoloans.(yearlist).(labelP{countP}).(labelT{countT});
    end

    %%NPV %
    NPVpercent.(labelP{countP}).(labelT{countT}) = 100*NPV.(labelP{countP}).(labelT{
(countT))./(TI.(labelP{countP}).(labelT{countT})*15);

    %%ROI calculation
    totalprofit.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
    for year = 4:18
        yearlist = ['year' num2str(year)];
        totalprofit.(labelP{countP}).(labelT{countT}) = totalprofit.(labelP{
(countP)).(labelT{countT}) +...
            cashflowBT.(yearlist).(labelP{countP}).(labelT{countT});
    end
    avgprofit.(labelP{countP}).(labelT{countT}) = totalprofit.(labelP{countP}).✓

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(labelT{countT})./15;
    ROIBT.(labelP{countP}).(labelT{countT}) = 100.*avgprofit.(labelP{countP}).✓
(labelT{countT})./TI.(labelP{countP}).(labelT{countT});
    %%IRR calculation
    %comment out fsolve for speed
    options = optimoptions(@fsolve,'DiffMaxChange',0.005,'FunctionTolerance',✓
0.01,'Display','off');
    rate = zeros(length(NPV.(labelP{countP}).(labelT{countT})),1);
    for z = 2:length(NPV.(labelP{countP}).(labelT{countT}))
        if NPV.(labelP{countP}).(labelT{countT})(z) < 2
            rate0 = -3;
        else
            rate0 = 0.1;
        end
        p.countT = countT;
        p.countP = countP;
        p.labelT = labelT;
        p.labelP = labelP;
        p.z = z;
        p.cashflow = cashflownoloans;
        % use IRR calculation
        %
            rate(z) = fsolve(@(rate) IRRsolver(rate,p),rate0,✓
options);
        % ignore IRR to speed up code
        rate(z) = 0;
        IRR.(labelP{countP}).(labelT{countT})(z) = rate(z);
    end
end
end

% for j = 10:5:30
%     P = j; %bar
%     countP = (j-10)/5 + 1;
%     for i = 300:20:380
%         countT = (i - 300)/20 + 1;
%         [maxes(countT),I1(countT)] = max(NPV.(labelP{countP}).(labelT{countT}));
%         maxes2(countT) = max(NPVpercent.(labelP{countP}).(labelT{countT}));
%         maxes3(countT) = max(IRR.(labelP{countP}).(labelT{countT}));
%     end
%     [maxNPV.(labelP{countP}),I] = max(maxes);
%     maxNPVpercent.(labelP{countP}) = max(maxes2);
%     maxIRR.(labelP{countP}) = max(maxes3);
%     % index.(labelP{countP}) = I1(I)
% end

% %cash flow diagram
% for year = 1:18
%     conversionindex = 25;
%     countT = 7;
%     yearlist = ['year' num2str(year)];

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```

%     yearlistprevious = ['year' num2str(year-1)];
%     CumDiscCashFlow(year) = CumulativeDiscountedCashFlowLoan.(yearlist).(labelP{
countP}).(labelT{countT})(conversionindex);
%     CumCashFlow(year) = CumulativeNonDiscountedCashFlowLoan.(yearlist).(labelP{
countP}).(labelT{countT})(conversionindex);
%     CumDiscCashFlowNoLoan(year) = CumulativeDiscountedCashFlowNoLoan.(yearlist).(
labelP{countP}).(labelT{countT})(conversionindex);
%     CumCashFlowNoLoan(year) = CumulativeNonDiscountedCashFlowNoLoan.(yearlist).(
labelP{countP}).(labelT{countT})(conversionindex);
% end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%-----plotting-----%
countP = 1;
for z=1
    figure1 = figure('Color',[1 1 1]);
    figure2 = figure('Color',[1 1 1]);
    figure3 = figure('Color',[1 1 1]);
    figure4 = figure('Color',[1 1 1]);
    figure5 = figure('Color',[1 1 1]);
    figure6 = figure('Color',[1 1 1]);
    figure7 = figure('Color',[1 1 1]);
    figure8 = figure('Color',[1 1 1]);
    figure9 = figure('Color',[1 1 1]);
    figure10 = figure('Color',[1 1 1]);
    figure11 = figure('Color',[1 1 1]);
    figure12 = figure('Color',[1 1 1]);
    figure13 = figure('Color',[1 1 1]);
    figure14 = figure('Color',[1 1 1]);
    figure15 = figure('Color',[1 1 1]);
    figure16 = figure('Color',[1 1 1]);
    figure17 = figure('Color',[1 1 1]);

    figure.figure1
    for i = 225:5:240
        countT = (i - 225)/5 + 1;
        hold on
        % plot mole fraction as function of tau
        plot(tau.(labelP{countP}).(labelT{countT})*60,Ethanol.(labelP{countP}).(labelT{
countT}),'Color',cc(countT,:),'LineWidth',1.5)
        xlabel('Residence Time [min]');ylabel('Molar Flow Rate Ethanol [gmol/hr]')
        %     axis([0 500 4 10])
    end
    axes1 = get(figure1,'CurrentAxes');
    hold(axes1,'on');
    box(axes1,'on');
    set(axes1,'FontWeight','bold');
    legend(['225' char(176) 'C'],['230' char(176) 'C'],['235' char(176) 'C'],...
        ['240' char(176) 'C'],'Location','NE','FontSize',11)

```



```

figure.figure2
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    %plot molar flow rate PEtA vs residence time
    hold on
    plot((tau.(labelP{countP}).(labelT{countT})).*60,EtA.(labelP{countP}).(labelT{
countT}),'Color',cc(countT,:),'LineWidth',1.5)
    xlabel('Residence Time [min]');ylabel('Molar Flow Rate Ethyl Acetate'
[gmol/hr]')
end
%    axis([0 500 0 2.2])
axes1 = get(figure2,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
legend(['225' char(176) 'C'],['230' char(176) 'C'],['235' char(176) 'C'],...
    ['240' char(176) 'C'],'Location','NE','FontSize',11)

figure.figure3
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    %
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),sEtA.(labelP{countP}).(labelT{
countT}),'Color',cc(countT,:),'LineWidth',1.5)
    xlabel('Ethanol Conversion');
    ylabel('Ethyl Acetate Selectivity')
end
%    axis([0 0.6 0.35 0.5])
axes1 = get(figure3,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%    yline = [-30:300]';
%    oppoint = 0.25;
%    plot(zeros(length(yline),1)+oppoint,'
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['225' char(176) 'C'],['230' char(176) 'C'],['235' char(176) 'C'],...
    ['240' char(176) 'C'],'Location','NE','FontSize',11)

%
figure.figure4
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),Revenue.(labelP{countP}).(labelT{
countT}),'Color',cc(countT,:),'LineWidth',1.5)
    xlabel('Ethanol Conversion');ylabel('Revenue [MM$]')
end
%    axis([0 0.6 25 40])

```

```

axes1 = get(figure4, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
%   ylabel = [-30:300]';
%   oppoint = 0.25;
%   plot(zeros(length(yline),1)+oppoint, ↵
ylabel, 'LineStyle', '--', 'Color', 'k', 'Linewidth', 1, 'Marker', 'none')
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'], ...
      ['240' char(176) 'C'], 'Location', 'NE', 'FontSize', 11)

%
figure(figure5)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), Vreal.(labelP{countP}).(labelT{↵
{countT})./1000, 'Color', cc(countT,:), 'LineWidth', 1.5)
    xlabel('Ethanol Conversion');
    ylabel('Reactor Volume [m^3]')
end
%   axis([0 0.6 0 3*10^3])
axes1 = get(figure5, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
%   ylabel = [-30:30000]';
%   oppoint = 0.25;
%   plot(zeros(length(yline),1)+oppoint, ↵
ylabel, 'LineStyle', '--', 'Color', 'k', 'Linewidth', 1, 'Marker', 'none')
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'], ...
      ['240' char(176) 'C'], 'Location', 'NE', 'FontSize', 11)

%
figure(figure7)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), (FEthanol.(labelP{countP}).(labelT{↵
{countT})-PEthanol.(labelP{countP}).(labelT{countT})), 'Color', cc(countT,:), 'LineWidth', ↵
1.5)
    xlabel('Ethanol Conversion'); ylabel('Fresh Feed Ethanol [gmol/hr]')
end
%   axis([0 0.6 160000 240000]);
axes1 = get(figure7, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
%   ylabel = [-30:300]';
%   oppoint = 0.25;

```

```

%      plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
    legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
        ['240' char(176) 'C'],'Location','NE','FontSize',11)

%
figure.figure9
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPV.(labelP{countP}).(labelT{↵
{countT}), 'Color',cc(countT,:), 'LineStyle','-', 'Marker','none', 'LineWidth',1.5)
    xlabel('Ethanol Conversion')
    ylabel('NPV_{project} [MM$]')
    %      axis([0 0.6 -100 90])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPVpercent.(labelP{countP}).(labelT{↵
{countT}), 'Color',cc(countT,:), 'LineStyle','-.', 'Marker','none', 'LineWidth',1.5)
    ylabel('NPV_%')
        axis([0 0.6 35 95])

end
axes1 = get(figure9, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
yyaxis left
axes1 = get(figure9, 'CurrentAxes');
set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
%      yline = [-300:300]';
%      oppoint = 0.25;
%      plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
    legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
        ['240' char(176) 'C'],'Location','NE','FontSize',11)

%
figure.figure10
for i = 240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),PEther.(labelP{countP}).(labelT{↵
{countT})./PTotal.(labelP{countP}).(labelT{countT}),...
        xt.(labelP{countP}).(labelT{countT}),PEtA*ones(length(xt.(labelP{countP}).↵
(labelT{countT}),1)./PTotal.(labelP{countP}).(labelT{countT}),...
        xt.(labelP{countP}).(labelT{countT}),PEthanol.(labelP{countP}).(labelT{↵
{countT})./PTotal.(labelP{countP}).(labelT{countT}), 'LineWidth',1.5)
    yline = [-30:300]';
    oppoint = 0.25;

```

```

%       plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
    legend('x_{Ether}','x_{Ethyl Acetate}','x_{↵
{Ethanol}','Location','best','FontSize',11)
    xlabel('Ethanol Conversion');
    ylabel('Reactor Effluent Mole Fraction')
end
%       axis([0 0.6 0 1])
axes1 = get(figure10,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');

%
figure(figure11)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(NPV.(labelP{countP}).(labelT{countT}),NPVpercent.(labelP{countP}).(labelT↵
{countT}), 'Color',cc(countT,:), 'LineWidth',1.5)
end
%       axis([40 80 0 30])
ylabel('NPV_%')
xlabel('NPV_{project} [MM$]')
axes1 = get(figure11,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
    ['240' char(176) 'C'], 'Location','NE','FontSize',11)

%
figure(figure12)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    IRRplot.(labelP{countP}).(labelT{countT}) = 100*IRR.(labelP{countP}).(labelT↵
{countT});
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),IRRplot.(labelP{countP}).(labelT↵
{countT}), 'Color',cc(countT,:), 'LineWidth',1.5)
end
%       axis([0 0.6 0 45])
ylabel('IRR [%]')
xlabel('Ethanol Conversion')
axes1 = get(figure12,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%       yline = [-30:300]';

```

```

%       oppoint = 0.25;
%       plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
       ['240' char(176) 'C'],'Location','NE','FontSize',11)

%
figure(figure13)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),ROI_BT.(labelP{countP}).(labelT{↵
{countT}),'Color',cc(countT,:), 'LineWidth',1.5)
end
%       axis([0 0.6 -10 70])
ylabel('ROI_{BT} [%]')
xlabel('Ethanol Conversion')
axes1 = get(figure13,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%       yline = [-30:300]';
%       oppoint = 0.25;
%       plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
       ['240' char(176) 'C'],'Location','NE','FontSize',11)

%
figure(figure14)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),TI.(labelP{countP}).(labelT{↵
{countT}),'Color',cc(countT,:), 'LineWidth',1.5)
end
%       axis([0 0.6 0 100])
ylabel('TCI [MM$]')
xlabel('Ethanol Conversion')
axes1 = get(figure14,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%       yline = [-30:300]';
%       oppoint = 0.25;
%       plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['225' char(176) 'C'], ['230' char(176) 'C'], ['235' char(176) 'C'],...
       ['240' char(176) 'C'],'Location','NE','FontSize',11)
%

```

```

figure(figure15)
for i = 240
    countT = (i - 225)/5 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),ROI_BT.(labelP{countP}).(labelT{countT}), 'Color','k','LineStyle','-','Marker','none','LineWidth',1.5)
    xlabel('Ethanol Conversion')
    ylabel('ROI_{BT} [%]')
    % axis([0 0.6 -10 70])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),TI.(labelP{countP}).(labelT{countT}), 'Color','k','LineStyle','-','Marker','none','LineWidth',1.5)
    ylabel('TCI [MM $]')
    % axis([0 0.6 0 100])
end
axes1 = get(figure15,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold','YColor','k');
yyaxis left
axes1 = get(figure15,'CurrentAxes');
set(axes1,'FontWeight','bold','YColor','k');
% yline = [-30:300]';
% oppoint = 0.25;
% plot(zeros(length(yline),1)+oppoint, yline, 'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['ROI_{BT}'], ['TI'], 'Location','NE', 'FontSize',11)

%
figure(figure6)
countP = 1;
for i = 240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),PEther.(labelP{countP}).(labelT{countT})./1000,...
        xt.(labelP{countP}).(labelT{countT}),PEtA*ones(1,length(xt.(labelP{countP}).(labelT{countT}))./1000,...
        xt.(labelP{countP}).(labelT{countT}),PEthanol.(labelP{countP}).(labelT{countT})./1000,'LineWidth',1.5)
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),FEthanol.(labelP{countP}).(labelT{countT})./1000,'LineWidth',1.5)
    plot(xt.(labelP{countP}).(labelT{countT}),FreshFeed.(labelP{countP}).(labelT{countT})./1000,'LineWidth',1.5)
    % yline = [-30:3000]';
    % oppoint = 0.25;

```

```

        %      plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
        legend('P_{Ether}','P_{Ethyl Acetate}','R_{Ethanol}','F_{Ethanol}','F_{Fresh↵
Ethanol}','Location','best','FontSize',11)
        xlabel('Toluene Conversion');ylabel('Molar Flowrate [kgmol/hr]')
        %      axis([0 0.6 0 10*max(PEtA)./1000])
        axes1 = get(figure6,'CurrentAxes');
        hold(axes1,'on');
        box(axes1,'on');
        set(axes1,'FontWeight','bold');
    end

figure(figure8)
%only one temp as PTotal is independent of temp for a given conversion
for i = 240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),PTotal.(labelP{countP}).(labelT↵
{countT}),'Color',cc(countT,:), 'LineWidth',1.5)
    xlabel('Ethanol Conversion');ylabel('Total Flow to Sep Unit [gmol/hr]')
    %      axis([0 0.6 0 1e7])
    axes1 = get(figure8,'CurrentAxes');
    hold(axes1,'on');
    box(axes1,'on');
    set(axes1,'FontWeight','bold');
    %      yline = [-30:30000000]';
    %      oppoint = 0.25;
    %      plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
end

%
figure(figure16)
countT = 4;
for j = 2:2:10
    P = j; %bar
    countP = (j-2)/2 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPV.(labelP{countP}).(labelT↵
{countT}),'Color',cc(countP,:), 'LineStyle','-', 'Marker','none', 'LineWidth',1.5)
    xlabel('Toluene Conversion')
    ylabel('NPV_{project} [MM$]')
    %      axis([0 0.6 -10 80])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPVpercent.(labelP{countP}).(labelT↵
{countT}),'Color',cc(countP,:), 'LineStyle','-.', 'Marker','none', 'LineWidth',1.5)

```

```

        ylabel('NPV_%')
        %           axis([0 0.6 0 30])
    end
    axes1 = get(figure16, 'CurrentAxes');
    hold(axes1, 'on');
    box(axes1, 'on');
    set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
    yyaxis left
    axes1 = get(figure16, 'CurrentAxes');
    set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
    %       ylabel = [-300:300]';
    %       oppoint = 0.25;
    %           plot(zeros(length(yline),1)+oppoint, ↵
ylabel, 'LineStyle', '--', 'Color', 'k', 'Linewidth', 1, 'Marker', 'none')
    %
    legend(['2 atm'], ['4 atm'], ...
        ['6 atm'], ['8 atm'], ['10 atm'], 'Location', 'NE', 'FontSize', 11)
    %
    %
    %           %
    figure(figure17)
    for j = 2:2:10
        P = j; %bar
        countP = (j-2)/2 + 1;
        hold on
        plot(xt.(labelP{countP}).(labelT{countT}), Vreal.(labelP{countP}).(labelT{countT})./1000, 'Color', cc(countP,:), 'LineWidth', 1.5)
        xlabel('Ethanol Conversion');
        ylabel('Reactor Volume [m^3]')
    end
    %       axis([0 0.6 0 3*10^3])
    axes1 = get(figure17, 'CurrentAxes');
    hold(axes1, 'on');
    box(axes1, 'on');
    set(axes1, 'FontWeight', 'bold');
    %       ylabel = [-30:30000]';
    %       oppoint = 0.25;
    %           plot(zeros(length(yline),1)+oppoint, ↵
ylabel, 'LineStyle', '--', 'Color', 'k', 'Linewidth', 1, 'Marker', 'none')
    legend('2 atm', '4 atm', '6 atm', '8 atm', '10 atm', 'Location', 'NE', 'FontSize', 11)

end
% ----- %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% toc

function F = IRRsolver(rate,p)

```



```
countP = p.countP;
countT = p.countT;
labelP = p.labelP;
labelT = p.labelT;
z = p.z;
cashflow = p.cashflow;
NPVIRR.(labelP{countP}).(labelT{countT})(z) = 0;
for year = 1:18
    yearlist = ['year' num2str(year)];
    discount.(yearlist) = (1/((1 + rate)^year));
    NPVIRRCashflow.(yearlist).(labelP{countP}).(labelT{countT}) = cashflow.(yearlist).✓
(labelP{countP}).(labelT{countT})(z).*discount.(yearlist);
    NPVIRR.(labelP{countP}).(labelT{countT})(z) = NPVIRR.(labelP{countP}).(labelT{✓
{countT})(z) + NPVIRRCashflow.(yearlist).(labelP{countP}).(labelT{countT});
end
F(1) = NPVIRR.(labelP{countP}).(labelT{countT})(z);
end
```

```
clear
close all
tic
%this script solves the concentration profiles in our isothermal ideal pfr
%neglecting pressure drop to determine the selectivities, toluene
%conversion, and molar flow streams for a desired production rate of
%para-xylene by toluene disproportionation

%additionally this script determines revenue from flow streams from the
%separated components, and calculates NPV, TCI, ROI, and IRR from cash
%flows
Price.EtA = 1100;[$/MT]
Price.Ethanol = 500;[$/MT]
Price.Fuel = 2.5;[$/MM BTU]
Price.Electricity = 0.08; % $/kw hr
Price.CO2 = 40; %$/MT
Price.Cat = 10000; %$/MT
MW.EtA = 88.11;[g/gmol]
MW.Ethanol = 46.07;[g/gmol]
MW.Acetaldehyde = 44.05;[g/gmol]
MW.Ether = 74.12;[g/gmol]
MW.H2 = 2.02;[g/gmol]

lambda.EtA = 38.0; %kJ/mol, latent heat of evaporation
lambda.Ethanol = 42.3; %kJ/mol, latent heat of evaporation
lambda.Ether = 33.8; %kJ/mol, latent heat of evaporation

Cp.EthanolGas = 74/1000; %kJ/mol*K
Cp.EthanolLiq = 118/1000; %kJ/mol*K

dHcomb.H2 = 286; % kJ/mol

MethaneEnergy = 891; %kJ/gmol
MethaneCarbon = 1; %kJ/gmol

EnterpriseRate = 0.1;
ConstructionInterestRate = 0.05;
IncomeTaxRate = 0.27;
FCImultiplier = 1;
SUMultiplier = 1;
WCMultiplier = 1;

% P = 10; %[atm]
R = 0.08206; %[L*atm/K*mol]
R = R*1.01325; %[L*bar/K*mol]
F = 50;[gmol/hr] basis flowrate used to solve system before scale up
PEtA = 67556; [gmol/hr]
Vmax = 10; %[L]
labelT = {'T225' 'T230' 'T235' 'T240'};
labelP = {'P2' 'P4' 'P6' 'P8' 'P10'};
```

```

cc=length(length(labelP));
for j = 2:2:10
    P = j; %bar
    countP = (j-2)/2 + 1;
    for i = 225:5:240
        countT = (i - 225)/5 + 1;
        T = i + 273;
        %assume reactor feed is pure toluene and equal to plant feed stream of
        %toluene
        Q = [1 0 0 0 0 0]*F; %feed molar flowrate in gmol/hr
        %solve ode
        resolution = 500;
        Vspan = [0 1.87 2.68 3.85 5.7 9.4];
        %           Vspan = logspace(-3,log10(Vmax),1001);
        opts = odeset('RelTol',1e-12,'AbsTol',1e-12);
        [Vout, Nout] = ode15s(@ (V,N) EtAcetateReactor_PBR_Ideal_184B(V,N,T,P),Vspan,Q,
opts);

        %store output of ode45 in structures containing all values at different
        %temperatures
        V.(labelP{countP}).(labelT{countT}) = Vout(2:end);
        Ethanol.(labelP{countP}).(labelT{countT}) = Nout(2:end,1);
        Acetaldehyde.(labelP{countP}).(labelT{countT}) = Nout(2:end,2);
        H2.(labelP{countP}).(labelT{countT}) = Nout(2:end,3);
        EtA.(labelP{countP}).(labelT{countT}) = Nout(2:end,4);
        Ether.(labelP{countP}).(labelT{countT}) = Nout(2:end,5);
        H2O.(labelP{countP}).(labelT{countT}) = Nout(2:end,6);

        %compute tau for all reactor sizes output from ode45
        for new = 1:length(V.(labelP{countP}).(labelT{countT}))
            tau.(labelP{countP}).(labelT{countT})(new,1) = Vout(new)*P./(R*T*sum(Nout
(new,:)));
        end
        %calculate selectivity and conversion for selected T and Ft
        Ft = F;
        xt.(labelP{countP}).(labelT{countT}) = (Ft - Ethanol.(labelP{countP}).(labelT
{countT}))./Ft;%reactor conversion of Ethanol
        sEtA.(labelP{countP}).(labelT{countT}) = EtA.(labelP{countP}).(labelT
{countT})./((1/l)*(Ft - Ethanol.(labelP{countP}).(labelT{countT})));%reactor
selectivity for EtA
        sEther.(labelP{countP}).(labelT{countT}) = Ether.(labelP{countP}).(labelT
{countT})./((1/l)*(Ft - Ethanol.(labelP{countP}).(labelT{countT})));%reactor
selectivity for Ether

        %calculate real molar feeds, volumetric flow, and total reactor volume
        %at full scale
        FEthanol.(labelP{countP}).(labelT{countT}) = PEtA./(xt.(labelP{countP}).(labelT
{countT})).*sEtA.(labelP{countP}).(labelT{countT}));%feed reate of Ethanol to reactor
for desired PEtA [gmol/hr]
        qreal.(labelP{countP}).(labelT{countT}) = R*T*FEthanol.(labelP{countP}).(labelT
{countT})/P;%real volumetric flowrate [L/hr]

```

```

Vreal.(labelP{countP}).(labelT{countT}) = tau.(labelP{countP}).(labelT{countT}).*qreal.(labelP{countP}).(labelT{countT});%real reactor total volume [L]

%calculate the product molar flowrates from full scale reactor
PEther.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT}).*xt.(labelP{countP}).(labelT{countT}).*sEther.(labelP{countP}).(labelT{countT});%Product molar flow Ether [gmol/hr]
PH2O.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{countT});
PEthanol.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT}).*(1-xt.(labelP{countP}).(labelT{countT}));%Product molar flow Ethanol [gmol/hr]
PH2.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT}) - PEthanol.(labelP{countP}).(labelT{countT});%Product molar flow Hydrogen [gmol/hr]
PTotal.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{countT})+PEthanol.(labelP{countP}).(labelT{countT})+PH2.(labelP{countP}).(labelT{countT})+PH2O.(labelP{countP}).(labelT{countT})+PEtA;

%create vectors of mass flowrates
PMEther.(labelP{countP}).(labelT{countT}) = PEther.(labelP{countP}).(labelT{countT}).*MW.Ether./(10^3);%[kg/hr]
PMEthanol.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{countT}).*MW.Ethanol./(10^3);%[kg/hr]
FMEthanol.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT}).*MW.Ethanol./(10^3);%[kg/hr]
PMEtA.(labelP{countP}).(labelT{countT}) = (PEtA*MW.EtA/(10^3)).*ones(length(PEthanol.(labelP{countP}).(labelT{countT})),1);%[kg/hr]

%calculate the fresh feed stream flowrate assuming perfect separations
FreshFeed.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT})-PEthanol.(labelP{countP}).(labelT{countT});
FreshFeedM.(labelP{countP}).(labelT{countT}) = FreshFeed.(labelP{countP}).(labelT{countT}).*MW.Ethanol./(10^3);%[kg/hr]

%%equipment costs
%reactor - sufficiently estimated with single tubular reactor cost
VR.(labelP{countP}).(labelT{countT}) = Vreal.(labelP{countP}).(labelT{countT})/1000; %m^3
VR.(labelP{countP}).(labelT{countT}) = VR.(labelP{countP}).(labelT{countT})*(3.28^3); %ft^3
Fm = 2.25; %stainless steel - H2 embrittlement
% pressure correction
if P < 3.45
    Fp = 1.00;
elseif P < 6.9
    Fp = 1.05;
elseif P < 13.8
    Fp = 1.15;
elseif P < 20.7

```

```

        Fp = 1.20;
elseif P < 27.6
    Fp = 1.35;
elseif P < 34.5
    Fp = 1.45;
end
Fc = Fm*Fp;
MS = 1650;
%set L:D ratio
D.(labelP{countP}).(labelT{countT}) = ((4/10)*(VR.(labelP{countP}).(labelT{countT}))/pi)).^(1/3); %ft
H.(labelP{countP}).(labelT{countT}) = 10*D.(labelP{countP}).(labelT{countT}); %ft
Area.(labelP{countP}).(labelT{countT}) = pi.*(D.(labelP{countP}).(labelT{countT})).^2; %ft^2
ReactorCost.(labelP{countP}).(labelT{countT}) = (MS/280)*101.9*(D.(labelP{countP}).(labelT{countT}))^1.066.*(H.(labelP{countP}).(labelT{countT}))^0.82*(2.18+Fc);
ReactorCost.(labelP{countP}).(labelT{countT}) = ReactorCost.(labelP{countP}).(labelT{countT})/1e6; %MM$/yr

% feed furnace
eff = 0.70; % typical furnace efficiency
bp.Ethanol = 8*P+70; %linear approximation from phase diagram
Tf1 = 25;
Tf2 = bp.Ethanol;
T01 = bp.Ethanol;
T02 = T - 273;
QH2.(labelP{countP}).(labelT{countT}) = (eff)*PH2.(labelP{countP}).(labelT{countT})*dHcomb.H2; %kJ/hr
Qtotal.(labelP{countP}).(labelT{countT}) = FEthanol.(labelP{countP}).(labelT{countT})*(lambda.Ethanol + ...
    (Tf2-Tf1)*Cp.EthanolLiq + (T02-T01)*Cp.EthanolGas); %kJ/hr
for c = 1:length(QH2.(labelP{countP}).(labelT{countT}))
    if QH2.(labelP{countP}).(labelT{countT})(c) > Qtotal.(labelP{countP}).(labelT{countT})(c)
        Qfurnace.(labelP{countP}).(labelT{countT})(c,1) = Qtotal.(labelP{countP}).(labelT{countT})(c);
        Qresid.(labelP{countP}).(labelT{countT})(c,1) = 0;
    elseif Qtotal.(labelP{countP}).(labelT{countT})(c) > QH2.(labelP{countP}).(labelT{countT})(c)
        Qfurnace.(labelP{countP}).(labelT{countT})(c,1) = QH2.(labelP{countP}).(labelT{countT})(c);
        Qresid.(labelP{countP}).(labelT{countT})(c,1) = Qtotal.(labelP{countP}).(labelT{countT})(c) - QH2.(labelP{countP}).(labelT{countT})(c);
    end
end
Qfurnace.(labelP{countP}).(labelT{countT}) = Qfurnace.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM BTU/hr

```

```

%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = H2carbon*PH2.✓
(labelP{countP}).(labelT{countT}); %gmol/hr
%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.✓
(labelP{countP}).(labelT{countT})*44.01/1000; %kg/hr
%      FurnaceCarbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.✓
(labelP{countP}).(labelT{countT})*(24*50*7)/1000; %MT/year
FurnaceCarbon.(labelP{countP}).(labelT{countT}) = zeros(length(QH2.(labelP{
countP}).(labelT{countT})),1); %no carbon production from H2 combustion
Fc = 1.5; %stainless steel
FurnaceCost.(labelP{countP}).(labelT{countT}) = (MS/280)*(5.07e3) ...
*(Qfurnace.(labelP{countP}).(labelT{countT}).^0.85)*(1.23+Fc); %$
FurnaceCost.(labelP{countP}).(labelT{countT}) = FurnaceCost.(labelP{countP}).✓
(labelT{countT})/1e6; %MM$

% feed heat exchangers
SteamTemp = 139; %50psig sat steam

for c = 1:length(QH2.(labelP{countP}).(labelT{countT}))
    if QH2.(labelP{countP}).(labelT{countT})(c) > Qtotal.(labelP{countP}).✓
(labelT{countT})(c)
        %heat exchanger 1:
        T01 = 25; %C
        Tf1(c,1) = Qresid.(labelP{countP}).(labelT{countT})(c)./(FEthanol.✓
(labelP{countP}).(labelT{countT})(c).*Cp.EthanolLiq);
        dTA = SteamTemp - T01; %inlet temp difference
        dTB(c,1) = SteamTemp - Tf1(c); %outlet temp difference
        %sensible heat
        FeedHeating.(labelP{countP}).(labelT{countT})(c,1) = Qresid.(labelP{
countP}).(labelT{countT})(c); %kJ/hr
        FeedHeatinghr.(labelP{countP}).(labelT{countT})(c,1) = FeedHeating.✓
(labelP{countP}).(labelT{countT})(c)*0.947817/1e6; %MM Btu/hr
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = FeedHeatinghr.✓
(labelP{countP}).(labelT{countT})(c)*Price.Fuel*0.7; %$/hr (from table E.1-1)
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = H1SteamCost.✓
(labelP{countP}).(labelT{countT})(c)*(24*7*50)/1e6; %MM$/yr
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = 0; %MM$/yr %✓
assume heat integration with feed effluent
    % will be ingnored as design includes HX integration
    dTlm(c,1) = (dTA - dTB(c))./(log(dTA./dTB(c))); %approximation for log✓
mean temp diff
    dTlm(c,1) = dTlm(c)*9/5 + 32; %F
    elseif Qtotal.(labelP{countP}).(labelT{countT})(c) > QH2.(labelP{countP}).✓
(labelT{countT})(c)
        dTlm(c,1) = 1;
        FeedHeatinghr.(labelP{countP}).(labelT{countT})(c,1) = 0;
        H1SteamCost.(labelP{countP}).(labelT{countT})(c,1) = 0; %MM$/yr %✓
assume heat integration with feed effluent
    end
end
end

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```

U = 150; %BTU/ft^2 F h
eta = 0.7;
A = (eta)*FeedHeatinghr.(labelP{countP}).(labelT{countT})*1e6./(U.*dTlm); %ft^2
Fm = 2.81; %material correction, stainless steel
Fd = 1; %design correction
if P < 20.7
    Fp = 0; %pressure correction
elseif P < 27.6
    Fp = 0.1;
elseif P < 55.2
    Fp = 0.25;
end
Fc = (Fd + Fp)*Fm;
HX1Q.(labelP{countP}).(labelT{countT}) = FeedHeating.(labelP{countP}).(labelT{
countT}); %kJ/hr
HXcost1.(labelP{countP}).(labelT{countT}) = (MS/280)*101.3*(A.^0.65)*(2.29+Fc); %$

HXcost.(labelP{countP}).(labelT{countT}) = HXcost1.(labelP{countP}).(labelT{
countT})/1e6; %MM$

HeatOPCost.(labelP{countP}).(labelT{countT}) = H1SteamCost.(labelP{countP}).(
labelT{countT}); %MM$ /yr

%%separation system
PSepTotal.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{
countT})+PH2O.(labelP{countP}).(labelT{countT})+PEtA;
XH2O.(labelP{countP}).(labelT{countT}) = PH2O.(labelP{countP}).(labelT{
countT})./PSepTotal.(labelP{countP}).(labelT{countT});
XEthanol.(labelP{countP}).(labelT{countT}) = PEthanol.(labelP{countP}).(labelT{
countT})./PSepTotal.(labelP{countP}).(labelT{countT});
XEtA.(labelP{countP}).(labelT{countT}) = PEtA./PSepTotal.(labelP{countP}).(
labelT{countT});

for y = 1:length(xt.(labelP{countP}).(labelT{countT}))
    %Aspen Plus data
    if xt.(labelP{countP}).(labelT{countT})(y) > 0.47
        Dist1Qc.(labelP{countP}).(labelT{countT})(y) = 5.46*3.6e6; %kJ/hr
        Dist1Qr.(labelP{countP}).(labelT{countT})(y) = 6.22*3.6e6; %kJ/hr
        Dist1Nreal.(labelP{countP}).(labelT{countT})(y) = 38;
        Dist1rhog.(labelP{countP}).(labelT{countT})(y) = 2.36;
        Dist1V.(labelP{countP}).(labelT{countT})(y) = 572549;
        Dist1MV.(labelP{countP}).(labelT{countT})(y) = 57.01357;
        Dist2Qc.(labelP{countP}).(labelT{countT})(y) = 3.72*3.6e6; %kJ/hr
        Dist2Qr.(labelP{countP}).(labelT{countT})(y) = 3.33*3.6e6; %kJ/hr
        Dist2Nreal.(labelP{countP}).(labelT{countT})(y) = 48;
        Dist2rhog.(labelP{countP}).(labelT{countT})(y) = 2.41;
        Dist2V.(labelP{countP}).(labelT{countT})(y) = 561793;
        Dist2MV.(labelP{countP}).(labelT{countT})(y) = 66.80337;
    elseif xt.(labelP{countP}).(labelT{countT})(y) > 0.42

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Dist1Qc.(labelP{countP}).(labelT{countT})(y) = 8.4*3.6e6; %kj/hr
Dist1Qr.(labelP{countP}).(labelT{countT})(y) = 9.58*3.6e6; %kj/hr
Dist1Nreal.(labelP{countP}).(labelT{countT})(y) = 28;
Dist1rhog.(labelP{countP}).(labelT{countT})(y) = 2.34;
Dist1V.(labelP{countP}).(labelT{countT})(y) = 881195;
Dist1MV.(labelP{countP}).(labelT{countT})(y) = 56.54484;
Dist2Qc.(labelP{countP}).(labelT{countT})(y) = 3.66*3.6e6; %kj/hr
Dist2Qr.(labelP{countP}).(labelT{countT})(y) = 3.28*3.6e6; %kj/hr
Dist2Nreal.(labelP{countP}).(labelT{countT})(y) = 43;
Dist2rhog.(labelP{countP}).(labelT{countT})(y) = 2.41;
Dist2V.(labelP{countP}).(labelT{countT})(y) = 553393;
Dist2MV.(labelP{countP}).(labelT{countT})(y) = 66.90638;
elseif xt.(labelP{countP}).(labelT{countT})(y) > 0.37
Dist1Qc.(labelP{countP}).(labelT{countT})(y) = 8.32*3.6e6; %kj/hr
Dist1Qr.(labelP{countP}).(labelT{countT})(y) = 9.5*3.6e6; %kj/hr
Dist1Nreal.(labelP{countP}).(labelT{countT})(y) = 33;
Dist1rhog.(labelP{countP}).(labelT{countT})(y) = 2.33;
Dist1V.(labelP{countP}).(labelT{countT})(y) = 876150;
Dist1MV.(labelP{countP}).(labelT{countT})(y) = 56.14021;
Dist2Qc.(labelP{countP}).(labelT{countT})(y) = 3.6*3.6e6; %kj/hr
Dist2Qr.(labelP{countP}).(labelT{countT})(y) = 3.25*3.6e6; %kj/hr
Dist2Nreal.(labelP{countP}).(labelT{countT})(y) = 42;
Dist2rhog.(labelP{countP}).(labelT{countT})(y) = 2.4;
Dist2V.(labelP{countP}).(labelT{countT})(y) = 547246;
Dist2MV.(labelP{countP}).(labelT{countT})(y) = 66.729;
elseif xt.(labelP{countP}).(labelT{countT})(y) > 0.32
Dist1Qc.(labelP{countP}).(labelT{countT})(y) = 8.28*3.6e6; %kj/hr
Dist1Qr.(labelP{countP}).(labelT{countT})(y) = 9.45*3.6e6; %kj/hr
Dist1Nreal.(labelP{countP}).(labelT{countT})(y) = 47;
Dist1rhog.(labelP{countP}).(labelT{countT})(y) = 2.31;
Dist1V.(labelP{countP}).(labelT{countT})(y) = 869659;
Dist1MV.(labelP{countP}).(labelT{countT})(y) = 56.24488;
Dist2Qc.(labelP{countP}).(labelT{countT})(y) = 3.99*3.6e6; %kj/hr
Dist2Qr.(labelP{countP}).(labelT{countT})(y) = 3.52*3.6e6; %kj/hr
Dist2Nreal.(labelP{countP}).(labelT{countT})(y) = 37;
Dist2rhog.(labelP{countP}).(labelT{countT})(y) = 2.4;
Dist2V.(labelP{countP}).(labelT{countT})(y) = 598337.6;
Dist2MV.(labelP{countP}).(labelT{countT})(y) = 67.65983;
elseif xt.(labelP{countP}).(labelT{countT})(y) > 0
Dist1Qc.(labelP{countP}).(labelT{countT})(y) = 18.6*3.6e6; %kj/hr
Dist1Qr.(labelP{countP}).(labelT{countT})(y) = 21.2*3.6e6; %kj/hr
Dist1Nreal.(labelP{countP}).(labelT{countT})(y) = 22;
Dist1rhog.(labelP{countP}).(labelT{countT})(y) = 2.29;
Dist1V.(labelP{countP}).(labelT{countT})(y) = 1947300;
Dist1MV.(labelP{countP}).(labelT{countT})(y) = 55.09084;
Dist2Qc.(labelP{countP}).(labelT{countT})(y) = 5.51*3.6e6; %kj/hr
Dist2Qr.(labelP{countP}).(labelT{countT})(y) = 4.57*3.6e6; %kj/hr
Dist2Nreal.(labelP{countP}).(labelT{countT})(y) = 55;
Dist2rhog.(labelP{countP}).(labelT{countT})(y) = 2.39;
Dist2V.(labelP{countP}).(labelT{countT})(y) = 796140;

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Dist2MV.(labelP{countP}).(labelT{countT})(y) = 66.729;

end

%distillation column 1
Dist1P = 1; %bar

%      Dist1MvFeed = xa.*MW.Ether + xb.*MW.Ethanol + xc.*MW.EtA + xd.*MW.Ether;
%      Dist1MvDist = xa.*MW.Ether./xa;
%      Dist1MvBottoms = (xb.*MW.Ethanol + xc.*MW.EtA + xd.*MW.Ether).*(1./
(xb+xc+xd));
%      Dist1lambdaD = lambda.Benzene; %latent heat of distillate mixture
%      Dist1lambdaB = (xb.*lambda.Tol + xc.*lambda.ParaX + xd.*lambda.TMB).*(1./
(xb+xc+xd)); %latent heat of bottoms mixture

Dist1DSattemp = 85; %deg C, BP of mixture estimate
Dist1BSattemp = 76.5; %deg C, BP of Ethyl acetate
Dist1CoolingWaterCoolTemp = 25; % deg C
Dist1CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg C
Dist1SteamTemp = 194; % deg C, 200 psia steam
Dist1dTlmD.(labelP{countP}).(labelT{countT}) = ...
((Dist1DSattemp - Dist1CoolingWaterCoolTemp) - (Dist1DSattemp -
Dist1CoolingWaterHotTemp))/...
log((Dist1DSattemp - Dist1CoolingWaterCoolTemp)/(Dist1DSattemp -
Dist1CoolingWaterHotTemp));
Dist1dTlmB.(labelP{countP}).(labelT{countT}) = (Dist1SteamTemp -
Dist1BSattemp);
Dist1UD = 800; %W/m^2 K
Dist1UD = Dist1UD*60*60/1000; %kJ/hr m^2 K
Dist1UB = 820; %W/m^2 K
Dist1UB = Dist1UB*60*60/1000; %kJ/hr m^2 K
Dist1AreaD.(labelP{countP}).(labelT{countT}) = Dist1Qc.(labelP{countP}).
(labelT{countT})./(Dist1UD.*Dist1dTlmD.(labelP{countP}).(labelT{countT})); %m^2
Dist1AreaB.(labelP{countP}).(labelT{countT}) = Dist1Qr.(labelP{countP}).
(labelT{countT})./(Dist1UB.*Dist1dTlmB.(labelP{countP}).(labelT{countT})); %m^2

Fd = 1;
P0 = 11; %bar
Fp = 0.10*(Dist1P-P0)./P0;
Fm = 1;
Fi = 1.38;
FD = 2.3;
ah = 0.65;
A0 = 93; %m^2
Dist1HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
(MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist1AreaD.(labelP{countP}).
(labelT{countT}))./A0).^ah);
Dist1HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
(MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist1AreaB.(labelP{countP}).
(labelT{countT}))./A0).^ah);

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%column
Ht = 60; %cm
Hmin = 3.*Ht; %cm
Dist1H.(labelP{countP}).(labelT{countT}) = Hmin + Ht.*Dist1Nreal.(labelP{countP}).(labelT{countT}); %cm
Dist1H.(labelP{countP}).(labelT{countT}) = Dist1H.(labelP{countP}).(labelT{countT})./100; %m
c0 = 439;
phi = 0.6;
rho1 = 870; %kg/m^3
rhog = Dist1rhog.(labelP{countP}).(labelT{countT}); %kg/m^3
DV = Dist1V.(labelP{countP}).(labelT{countT});
Mv = Dist1MV.(labelP{countP}).(labelT{countT});
DistArea = (Mv./sqrt(rho1.*rhog))*(1./(phi.*c0)).*(.1./0.8).*DV;
Diameter = 2.*sqrt(DistArea./pi);
Fm = 1;
P0 = 4.5; %bar
t_p = 0.13*(Dist1P-P0)./P0;
Fp = 1+t_p*(1+exp(-t_p./2));
Fi = 1.38;
Fd = 3;
Fs = 1; % (for 60 cm tray spacing)
Ft = 0; %sieve
Dist1D.(labelP{countP}).(labelT{countT}) = Diameter;
d0 = 1; %m
H0 = 6.1; %m
as = 0.82;
at = 1.8;
CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(Dist1D.(labelP{countP}).(labelT{countT})./d0).*((Dist1H.(labelP{countP}).(labelT{countT})./H0).^as); %$
CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*((Dist1D.(labelP{countP}).(labelT{countT})./d0).^at).*(Dist1H.(labelP{countP}).(labelT{countT})./H0); %$
Dist1ColumnCost.(labelP{countP}).(labelT{countT}) = (CostShell + CostTray)/10; %$

Dist1QcBTU.(labelP{countP}).(labelT{countT}) = Dist1Qc.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
Dist1HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist1QcBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*1.13; %$/hr
Dist1HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist1HXDOpCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr

Dist1QrBTU.(labelP{countP}).(labelT{countT}) = Dist1Qr.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
Dist1HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist1QrBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*0.93; %$/hr
Dist1HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist1HXBOPCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr

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%distillation column 2
Dist2P = 20; %bar

%      Dist2MvFeed = xa.*MW.Ethanol + xb.*MW.EtA + xc.*MW.Ether;
%      Dist2MvDist = xa.*MW.Ethanol./xa;
%      Dist2MvBottoms = (xb.*MW.EtA + xc.*MW.Ether).*(1./(xb+xc));

%      Dist2lambdaD = lambda.Tol; %latent heat of distillate mixture
%      Dist2lambdaB = (xb.*lambda.ParaX + xc.*lambda.TMB).*(1./(xb+xc)); %latent
heat of bottoms mixture

Dist2DSattemp = 80; %deg C, BP of mixture, estimate
Dist2BSattemp = 90; %deg C, BP of bottoms mixture, estimate
Dist2CoolingWaterCoolTemp = 25; % deg C
Dist2CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg C
Dist2SteamTemp = 194; % deg C, 200 psia steam
Dist2dTlmD.(labelP{countP}).(labelT{countT}) = ...
    ((Dist2DSattemp - Dist2CoolingWaterCoolTemp) - (Dist2DSattemp -
Dist2CoolingWaterHotTemp))/...
    log((Dist2DSattemp - Dist2CoolingWaterCoolTemp)/(Dist2DSattemp -
Dist2CoolingWaterHotTemp));
Dist2dTlmB.(labelP{countP}).(labelT{countT}) = (Dist2SteamTemp -
Dist2BSattemp);
Dist2UD = 800; %W/m^2 K
Dist2UD = Dist2UD*60*60/1000; %kJ/hr m^2 K
Dist2UB = 820; %W/m^2 K
Dist2UB = Dist2UB*60*60/1000; %kJ/hr m^2 K
Dist2AreaD.(labelP{countP}).(labelT{countT}) = Dist2Qc.(labelP{countP}).
(labelT{countT})./(Dist2UD.*Dist2dTlmD.(labelP{countP}).(labelT{countT})); %m^2
Dist2AreaB.(labelP{countP}).(labelT{countT}) = Dist2Qr.(labelP{countP}).
(labelT{countT})./(Dist2UB.*Dist2dTlmB.(labelP{countP}).(labelT{countT})); %m^2

Fd = 1;
P0 = 11; %bar
Fp = 0.10*(Dist2P-P0)./P0;
Fm = 1;
Fi = 1.38;
FD = 2.3;
ah = 0.65;
A0 = 93; %m^2
Dist2HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
    (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist2AreaD.(labelP{countP}).
(labelT{countT})./A0).^ah);
Dist2HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
    (MS./301).*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist2AreaB.(labelP{countP}).
(labelT{countT})./A0).^ah);

Ht = 60; %cm

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Hmin = 3.*Ht; %cm
Dist2H.(labelP{countP}).(labelT{countT}) = Hmin + Ht.*Dist1Nreal.(labelP{countP}).(labelT{countT}); %cm
Dist2H.(labelP{countP}).(labelT{countT}) = Dist2H.(labelP{countP}).(labelT{countT})./100; %m
c0 = 439;
phi = 0.6;
rho1 = 870; %kg/m^3
rhog = Dist2rhog.(labelP{countP}).(labelT{countT}); %kg/m^3
DV = Dist2V.(labelP{countP}).(labelT{countT});
Mv = Dist2MV.(labelP{countP}).(labelT{countT});
DistArea = (Mv./sqrt(rho1.*rhog))*(1./(phi.*c0)).*(.1./0.8).*DV;
Diameter = 2.*sqrt(DistArea./pi);
Fm = 1;
P0 = 4.5; %bar
t_p = 0.13*(Dist2P-P0)./P0;
Fp = 1+t_p*(1+exp(-t_p./2));
Fi = 1.38;
Fd = 3;
Fs = 1; % (for 60 cm tray spacing)
Ft = 0; %sieve
Dist2D.(labelP{countP}).(labelT{countT}) = Diameter;
d0 = 1; %m
H0 = 6.1; %m
as = 0.82;
at = 1.8;
CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(Dist2D.(labelP{countP}).(labelT{countT})./d0).*((Dist2H.(labelP{countP}).(labelT{countT})./H0).^as); %$
CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*(Dist2D.(labelP{countP}).(labelT{countT})./d0).^at).*((Dist2H.(labelP{countP}).(labelT{countT})./H0); %$
Dist2ColumnCost.(labelP{countP}).(labelT{countT}) = (CostShell + CostTray)/10; %$

Dist2QcBTU.(labelP{countP}).(labelT{countT}) = Dist2Qc.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
Dist2HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist2QcBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*1.13; %$/hr
Dist2HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist2HXDOpCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr

Dist2QrBTU.(labelP{countP}).(labelT{countT}) = Dist2Qr.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
Dist2HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist2QrBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*0.93; %$/hr
Dist2HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist2HXBOPCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr

% distillation column 3
% Dist3P = 20; %bar
%
```

```

% %      MvFeed = xa.*MW.EtA + xb.*MW.Ether;
% %      MvDist = xa.*MW.EtA./xa;
% %      MvBottoms = xb.*MW.Ether./xb;
%
%      Dist3DSattemp = 78; %deg C, BP of Ethanol
%      Dist3BSattemp = 100; %deg C, BP of water
%      Dist3CoolingWaterCoolTemp = 25; % deg C
%      Dist3CoolingWaterHotTemp = Dist1CoolingWaterCoolTemp + 15; % deg C
%      Dist3SteamTemp = 194; % deg C, 200 psia steam
%      Dist1dTlmD.(labelP{countP}).(labelT{countT}) = ...
%          ((Dist3DSattemp - Dist3CoolingWaterCoolTemp) - (Dist3DSattemp -
Dist3CoolingWaterHotTemp))/...
%          log((Dist3DSattemp - Dist3CoolingWaterCoolTemp)/(Dist3DSattemp -
Dist3CoolingWaterHotTemp));
%      Dist3dTlmB.(labelP{countP}).(labelT{countT}) = (Dist3SteamTemp -
Dist3BSattemp);
%      Dist3UD = 770; %W/m^2 K
%      Dist3UD = Dist3UD*60*60/1000; %kJ/hr m^2 K
%      Dist3UB = 820; %W/m^2 K
%      Dist3UB = Dist3UB*60*60/1000; %kJ/hr m^2 K
%      Dist3AreaD.(labelP{countP}).(labelT{countT}) = Dist3Qc.(labelP{countP}).
(labelT{countT})./(Dist3UD.*Dist2dTlmD.(labelP{countP}).(labelT{countT})); %m^2
%      Dist3AreaB.(labelP{countP}).(labelT{countT}) = Dist3Qr.(labelP{countP}).
(labelT{countT})./(Dist3UB.*Dist2dTlmB.(labelP{countP}).(labelT{countT})); %m^2
%
%      Fd = 1;
%      P0 = 11; %bar
%      Fp = 0.10*(Dist3P-P0)./P0;
%      Fm = 1;
%      Fi = 1.38;
%      FD = 2.3;
%      ah = 0.65;
%      A0 = 93; %m^2
%      Dist3HXDCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301)*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist3AreaD.(labelP
{countP}).(labelT{countT})./A0).^ah);
%      Dist3HXBCost.(labelP{countP}).(labelT{countT}) = ... %$
%          (MS./301)*((Fd+Fp).*Fm-1+Fi.*FD).*8700.*((Dist3AreaB.(labelP
{countP}).(labelT{countT})./A0).^ah);
%
%
%      Ht = 60; %cm
%      Hmin = 3.*Ht; %cm
%      Dist3H.(labelP{countP}).(labelT{countT}) = Hmin + Ht.*Dist1Nreal.(labelP
{countP}).(labelT{countT}); %cm
%      Dist3H.(labelP{countP}).(labelT{countT}) = Dist3H.(labelP{countP}).
(labelT{countT})./100; %m
%      c0 = 439;
%      phi = 0.6;
%      rho1 = 870; %kg/m^3

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```

%      rhog = 1; %kg/m^3
%      Area = (Mv./sqrt(rhol.*rhog))*(1./(phi.*c0)).*(.1./0.8).*V;
%      Diameter = 2.*sqrt(Area./pi);
%      Fm = 1;
%      P0 = 4.5; %bar
%      t_p = 0.13*(Dist3P-P0)./P0;
%      Fp = 1+t_p*(1+exp(-t_p./2));
%      Fi = 1.38;
%      Fd = 3;
%      Fs = 1; % (for 60 cm tray spacing)
%      Ft = 0; %sieve
%      Dist3D.(labelP{countP}).(labelT{countT}) = Diameter;
%      d0 = 1; %m
%      H0 = 6.1; %m
%      as = 0.82;
%      at = 1.8;
%      CostShell = (MS./301).*(Fm.*Fp -1+Fi.*Fd).*5000.*(Dist3D.(labelP{countP}).(labelT{countT})./d0).*((Dist3H.(labelP{countP}).(labelT{countT})./H0).^as); %$
%      CostTray = (MS./301).*(Fs + Ft + Fm).*5000.*((Dist3D.(labelP{countP}).(labelT{countT})./d0).^at).*(Dist3H.(labelP{countP}).(labelT{countT})./H0); %$
%      Dist3ColumnCost.(labelP{countP}).(labelT{countT}) = (CostShell + CostTray)/10; %$
%
%      Dist3QcBTU.(labelP{countP}).(labelT{countT}) = Dist3Qc.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
%      Dist3HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist3QcBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*1.13; %$/hr
%      Dist3HXDOpCost.(labelP{countP}).(labelT{countT}) = Dist3HXDOpCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%
%      Dist3QrBTU.(labelP{countP}).(labelT{countT}) = Dist3Qr.(labelP{countP}).(labelT{countT})*0.947817/1e6; %MM Btu/hr
%      Dist3HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist3QrBTU.(labelP{countP}).(labelT{countT})*Price.Fuel*0.93; %$/hr
%      Dist3HXBOPCost.(labelP{countP}).(labelT{countT}) = Dist3HXBOPCost.(labelP{countP}).(labelT{countT})*(24*7*50)/1e6; %MM$/yr
%
%
%Sum of all three columns
DistSteamEnergy.(labelP{countP}).(labelT{countT}) = ... %kJ/hr
    Dist1Qr.(labelP{countP}).(labelT{countT}) + ...
    Dist2Qr.(labelP{countP}).(labelT{countT});
DistCost.(labelP{countP}).(labelT{countT}) = ... $
    Dist1HXDCost.(labelP{countP}).(labelT{countT}) + ...
    Dist1HXBCost.(labelP{countP}).(labelT{countT}) + ...
    Dist2HXDCost.(labelP{countP}).(labelT{countT}) + ...
    Dist2HXBCost.(labelP{countP}).(labelT{countT}) + ...
    Dist1ColumnCost.(labelP{countP}).(labelT{countT}) + ...
    Dist2ColumnCost.(labelP{countP}).(labelT{countT});

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        DistCost.(labelP{countP}).(labelT{countT}) = DistCost.(labelP{countP}).(labelT{countT})/1e6; %MM$
        DistOpCost.(labelP{countP}).(labelT{countT}) = ...
            Dist1HXDOpCost.(labelP{countP}).(labelT{countT}) + ...
            Dist2HXDOpCost.(labelP{countP}).(labelT{countT});
            Dist1HXBOPCost.(labelP{countP}).(labelT{countT}) + ...
            Dist2HXBOPCost.(labelP{countP}).(labelT{countT});
    end
    DistCost.(labelP{countP}).(labelT{countT}) = DistCost.(labelP{countP}).(labelT{countT})';
    DistOpCost.(labelP{countP}).(labelT{countT}) = DistOpCost.(labelP{countP}).(labelT{countT})';
    DistSteamEnergy.(labelP{countP}).(labelT{countT}) = DistSteamEnergy.(labelP{countP}).(labelT{countT})';
    % DistCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring cost
    % DistOpCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring operating cost
    % DistSteamEnergy.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring cost %kJ/hr

    %turbine
    gamma = 0.23;
    Pin = 1*2116.22; %lbf/ft^2
    Pout = P*2116.22; %lbf/ft^2
    Qin = (1/60)*0.0353147.*PTotal.(labelP{countP}).(labelT{countT})*R*300/1; %ft^3/min
    hp = (3.03e-5/gamma)*Pin.*Qin*((Pout/Pin)^gamma - 1);
    bhp = hp/0.8;
    Fd = 1.15; %reciprocal, turbine
    Fc = Fd;
    TurbCost.(labelP{countP}).(labelT{countT}) = (MS/280)*517.5*(bhp.^0.82)*(2.11 + Fc);
    TurbCost.(labelP{countP}).(labelT{countT}) = TurbCost.(labelP{countP}).(labelT{countT})/1e6;
    TurbCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
    %turbine operating costs
    TurbOPCost.(labelP{countP}).(labelT{countT}) = -(bhp/0.9)*(1/1.341)*Price*Electricity*8400/1e6; % MM$/year
    TurbOPCost.(labelP{countP}).(labelT{countT}) = zeros(length(A),1); %ignoring operating cost due to gained electricity powering pumps

    %carbon operating costs
    ElectricityCarbon.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
    SteamEnergy.(labelP{countP}).(labelT{countT}) = HX1Q.(labelP{countP}).(labelT{countT}) + DistSteamEnergy.(labelP{countP}).(labelT{countT}); %kJ/hr
    FlowMethaneForSteam.(labelP{countP}).(labelT{countT}) = SteamEnergy.(labelP{countP}).(labelT{countT})/MethaneEnergy; %gmol/hr
    SteamCarbon.(labelP{countP}).(labelT{countT}) = FlowMethaneForSteam.(labelP{countP}).(labelT{countT}); %gmol/hr

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    SteamCarbon.(labelP{countP}).(labelT{countT}) = SteamCarbon.(labelP{countP}).(
(labelT{countT})*44.01/1000; %kg/hr
    SteamCarbon.(labelP{countP}).(labelT{countT}) = SteamCarbon.(labelP{countP}).(
(labelT{countT})*(24*50*7)/1000; %MT/year
    Carbon.(labelP{countP}).(labelT{countT}) = FurnaceCarbon.(labelP{countP}).(
(labelT{countT}) + ...
        ElectricityCarbon.(labelP{countP}).(labelT{countT}) + ...
        SteamCarbon.(labelP{countP}).(labelT{countT}); %including carbon costs, $
    CarbonCost.(labelP{countP}).(labelT{countT}) = Carbon.(labelP{countP}).(labelT
(countT))*Price.CO2/1e6; %MM$
    %           CarbonCost.(label{count}) = zeros(length(A),1); %ignoring carbon
costs

    % total upfront equipment costs
    Equip.(labelP{countP}).(labelT{countT}) = HXcost.(labelP{countP}).(labelT
(countT)) + ...
        ReactorCost.(labelP{countP}).(labelT{countT}) + DistCost.(labelP{countP}).(
(labelT{countT}) + ...
        TurbCost.(labelP{countP}).(labelT{countT}) + FurnaceCost.(labelP{countP}).(
(labelT{countT})); %MM$
    FCI.(labelP{countP}).(labelT{countT}) = 2.28*Equip.(labelP{countP}).(labelT
(countT)); %MM$
    FCI.(labelP{countP}).(labelT{countT}) = FCImultiplier*FCI.(labelP{countP}).(
(labelT{countT})); %MM$ (for sensitivityanalysis)
    SU.(labelP{countP}).(labelT{countT}) = 0.1*FCI.(labelP{countP}).(labelT
(countT)); %MM$
    SU.(labelP{countP}).(labelT{countT}) = SUMultiplier*SU.(labelP{countP}).(labelT
(countT)); %MM$ (for sensitivityanalysis)
    WC.(labelP{countP}).(labelT{countT}) = 2/12*FreshFeedM.(labelP{countP}).(labelT
(countT))*Price.Ethanol/1000*24*7*50/1e6; %MM$/year
    WC.(labelP{countP}).(labelT{countT}) = WCMultiplier*WC.(labelP{countP}).(labelT
(countT)); %MM$ (for sensitivityanalysis)
    TI.(labelP{countP}).(labelT{countT}) = FCI.(labelP{countP}).(labelT{countT}) +
SU.(labelP{countP}).(labelT{countT}) + WC.(labelP{countP}).(labelT{countT}); %MM$

    %loan amount
    loan.(labelP{countP}).(labelT{countT}) = TI.(labelP{countP}).(labelT{countT});
    %construction rate for first 2 years, 2% higher than corporate rate
    ConstructionInterest.(labelP{countP}).(labelT{countT}) = loan.(labelP{countP}).(
(labelT{countT})*(ConstructionInterestRate);

    %corporate bond cash flows, 3% (DOW/BASF), total amount of construction
    %costs and interest up to that point, 10 year bond life (simple
    %interest)
    bond.(labelP{countP}).(labelT{countT}) = loan.(labelP{countP}).(labelT{countT})
+ ConstructionInterest.(labelP{countP}).(labelT{countT}) + ...
        ConstructionInterest.(labelP{countP}).(labelT{countT})*(1.05);
    CorporateInterest.(labelP{countP}).(labelT{countT}) = bond.(labelP{countP}).(
(labelT{countT})*(0.03);

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%chemical revenue, operating costs, and total revenuebefore taxes
Revenue.(labelP{countP}).(labelT{countT}) = (24*7*50)*(PMEtA.(labelP{countP}).✓
(labelT{countT})).*Price.EtA + ...
PMEthanol.(labelP{countP}).(labelT{countT})).*Price.Ethanol- FMEthanol.✓
(labelP{countP}).(labelT{countT})).*Price.Ethanol)/(1e9); %MM$/yr
RevenueProducts.(labelP{countP}).(labelT{countT}) = (24*7*50)*(PMEtA.(labelP✓
{countP}).(labelT{countT})).*Price.EtA)/1e9; %MM$/yr
AGS.(labelP{countP}).(labelT{countT}) = 0.1*RevenueProducts.(labelP{countP}).✓
(labelT{countT});
OperateCost.(labelP{countP}).(labelT{countT}) = DistOpCost.(labelP{countP}).✓
(labelT{countT}) + ...
HeatOPCost.(labelP{countP}).(labelT{countT}) + TurbOPCost.(labelP{countP}).✓
(labelT{countT}) + ...
CarbonCost.(labelP{countP}).(labelT{countT});
% cost of manufacturing
COM.(labelP{countP}).(labelT{countT}) = OperateCost.(labelP{countP}).(labelT✓
{countT}) + AGS.(labelP{countP}).(labelT{countT});

%salvage value, assuming 1% of initial equipment costs
salvage.(labelP{countP}).(labelT{countT}) = Equip.(labelP{countP}).(labelT✓
{countT})*0.01/2;

%depreciation, linear over 10 years
deprec.(labelP{countP}).(labelT{countT}) = (FCI.(labelP{countP}).(labelT✓
{countT}) + SU.(labelP{countP}).(labelT{countT}) ...
- salvage.(labelP{countP}).(labelT{countT}))./10; %/year
tax = IncomeTaxRate;

%%calculate cash flows
%assign initial cash flows, assuming 60/40 split during construction
cashflow.year1.(labelP{countP}).(labelT{countT}) = zeros(length(A),1) + loan.✓
(labelP{countP}).(labelT{countT}); %land
cashflow.year2.(labelP{countP}).(labelT{countT}) = -(0.6)*FCI.(labelP{countP}).✓
(labelT{countT});
%startup capital
cashflow.year3.(labelP{countP}).(labelT{countT}) = -(0.4)*FCI.(labelP{countP}).✓
(labelT{countT}) - SU.(labelP{countP}).(labelT{countT}) - ...
WC.(labelP{countP}).(labelT{countT}) - ConstructionInterest.(labelP✓
{countP}).(labelT{countT});
%cashflows during 10 year depreciation and corporate bond period
for year = 4:12
    yearlist = ['year' num2str(year)];
    profit.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP✓
{countP}).(labelT{countT}) - ...
    COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP✓
{countP}).(labelT{countT}) - ...
    deprec.(labelP{countP}).(labelT{countT}));
    cashflow.(yearlist).(labelP{countP}).(labelT{countT}) = (Revenue.(labelP✓
{countP}).(labelT{countT}) - ...
    COM.(labelP{countP}).(labelT{countT}) - CorporateInterest.(labelP✓

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(countP)).(labelT(countT)) - ...
    deprec.(labelP(countP)).(labelT(countT)).*(1-tax) + ...
    deprec.(labelP(countP)).(labelT(countT));
end
cashflow.year13.(labelP(countP)).(labelT(countT)) = Revenue.(labelP(countP)).✓
(labelT(countT)) - ...
    COM.(labelP(countP)).(labelT(countT)) - CorporateInterest.(labelP(countP)).✓
(labelT(countT)) - ...
    loan.(labelP(countP)).(labelT(countT));
%after depreciation and bond life
for year = 14:18
    yearlist = ['year' num2str(year)];
    cashflow.(yearlist).(labelP(countP)).(labelT(countT)) = (Revenue.(labelP✓
(countP)).(labelT(countT)) - ...
        COM.(labelP(countP)).(labelT(countT)).*(1-tax);
end
% Before tax cash flows
for year = 4:13
    yearlist = ['year' num2str(year)];
    cashflowBT.(yearlist).(labelP(countP)).(labelT(countT)) = (Revenue.(labelP✓
(countP)).(labelT(countT)) - ...
        COM.(labelP(countP)).(labelT(countT)) - CorporateInterest.(labelP✓
(countP)).(labelT(countT)));
end
for year = 14:18
    yearlist = ['year' num2str(year)];
    cashflowBT.(yearlist).(labelP(countP)).(labelT(countT)) = (Revenue.(labelP✓
(countP)).(labelT(countT)) - ...
        COM.(labelP(countP)).(labelT(countT)));
end

%salvage costs
cashflow.year18.(labelP(countP)).(labelT(countT)) = cashflow.year18.(labelP✓
(countP)).(labelT(countT)) + ...
    salvage.(labelP(countP)).(labelT(countT)) + WC.(labelP(countP)).(labelT✓
(countT));
%catalyst costs every 2 years
CatalystVol.(labelP(countP)).(labelT(countT)) = Vreal.(labelP(countP)).(labelT✓
(countT))*1000; %mL
CatalystMass.(labelP(countP)).(labelT(countT)) = CatalystVol.(labelP(countP)).✓
(labelT(countT))*0.5*6.31/1e6; %MT
CatalystCost.(labelP(countP)).(labelT(countT)) = CatalystMass.(labelP(countP)).✓
(labelT(countT))*Price.Cat/1e6; %MM$
for year = 3:1:18
    yearlist = ['year' num2str(year)];
    cashflow.(yearlist).(labelP(countP)).(labelT(countT)) = cashflow.✓
(yearlist).(labelP(countP)).(labelT(countT)) - ...
        CatalystCost.(labelP(countP)).(labelT(countT))*2;
end
cashflownoloans = cashflow;

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    cashflownoloans.year1.(labelP{countP}).(labelT{countT}) = cashflownoloans.✓
year1.(labelP{countP}).(labelT{countT}) - loan.(labelP{countP}).(labelT{countT});
    cashflownoloans.year13.(labelP{countP}).(labelT{countT}) = cashflownoloans.✓
year13.(labelP{countP}).(labelT{countT}) + loan.(labelP{countP}).(labelT{countT});
    %%NPV calculation
    NPV.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
    for year = 1:18
        yearlist = ['year' num2str(year)];
        discount.(yearlist) = (1/((1+EnterpriseRate)^year));
        NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT}) = cashflow.✓
(yearlist).(labelP{countP}).(labelT{countT}).*discount.(yearlist);
        NPVcashflownoloan.(yearlist).(labelP{countP}).(labelT{countT}) =✓
cashflownoloans.(yearlist).(labelP{countP}).(labelT{countT}).*discount.(yearlist);
        NPV.(labelP{countP}).(labelT{countT}) = NPV.(labelP{countP}).(labelT{✓
countT}) + NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT});
    end
    % cumulative cash flows
    CumulativeDiscountedCashFlowLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeDiscountedCashFlowNoLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeNonDiscountedCashFlowLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);
    CumulativeNonDiscountedCashFlowNoLoan.year0.(labelP{countP}).(labelT{countT}) =✓
zeros(length(A),1);

    for year = 1:18
        yearlist = ['year' num2str(year)];
        yearlistprevious = ['year' num2str(year-1)];
        CumulativeDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{✓
countT}) = ...
            CumulativeDiscountedCashFlowLoan.(yearlistprevious).(labelP{countP}).✓
(labelT{countT}) ...
            + NPVcashflow.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{✓
countT}) = ...
            CumulativeDiscountedCashFlowNoLoan.(yearlistprevious).(labelP{countP}).✓
(labelT{countT}) ...
            + NPVcashflownoloan.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeNonDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{✓
countT}) = ...
            CumulativeNonDiscountedCashFlowLoan.(yearlistprevious).(labelP{✓
countP}).(labelT{countT}) ...
            + cashflow.(yearlist).(labelP{countP}).(labelT{countT});
        CumulativeNonDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{✓
countT}) = ...
            CumulativeNonDiscountedCashFlowNoLoan.(yearlistprevious).(labelP{✓
countP}).(labelT{countT}) ...
            + cashflownoloans.(yearlist).(labelP{countP}).(labelT{countT});
    end

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%%NPV %
NPVpercent.(labelP{countP}).(labelT{countT}) = 100*NPV.(labelP{countP}).(labelT{countT})./(TI.(labelP{countP}).(labelT{countT})*15);

%%ROI calculation
totalprofit.(labelP{countP}).(labelT{countT}) = zeros(length(A),1);
for year = 4:18
    yearlist = ['year' num2str(year)];
    totalprofit.(labelP{countP}).(labelT{countT}) = totalprofit.(labelP{countP}).(labelT{countT}) + ...
        cashflowBT.(yearlist).(labelP{countP}).(labelT{countT});
end
avgprofit.(labelP{countP}).(labelT{countT}) = totalprofit.(labelP{countP}).(labelT{countT})./15;
ROIBT.(labelP{countP}).(labelT{countT}) = 100.*avgprofit.(labelP{countP}).(labelT{countT})./TI.(labelP{countP}).(labelT{countT});
%%IRR calculation
%comment out fsolve for speed
options = optimoptions(@fsolve,'DiffMaxChange',0.005,'FunctionTolerance',0.01,'Display','off');
rate = zeros(length(NPV.(labelP{countP}).(labelT{countT})),1);
for z = 2:length(NPV.(labelP{countP}).(labelT{countT}))
    if NPV.(labelP{countP}).(labelT{countT})(z) < 2
        rate0 = -3;
    else
        rate0 = 0.1;
    end
    p.countT = countT;
    p.countP = countP;
    p.labelT = labelT;
    p.labelP = labelP;
    p.z = z;
    p.cashflow = cashflownoloans;
    % use IRR calculation
    rate(z) = fsolve(@(rate) IRRsolver(rate,p),rate0,options);
    % ignore IRR to speed up code
    rate(z) = 0;
    IRR.(labelP{countP}).(labelT{countT})(z) = rate(z);
end
end
end

% for j = 10:5:30
%     P = j; %bar
%     countP = (j-10)/5 + 1;
%     for i = 300:20:380
%         countT = (i - 300)/20 + 1;
%         [maxes(countT),I1(countT)] = max(NPV.(labelP{countP}).(labelT{countT}));

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%      maxes2(countT) = max(NPVpercent.(labelP{countP}).(labelT{countT}));
%      maxes3(countT) = max(IRR.(labelP{countP}).(labelT{countT}));
%      end
%      [maxNPV.(labelP{countP}),I] = max(maxes);
%      maxNPVpercent.(labelP{countP}) = max(maxes2);
%      maxIRR.(labelP{countP}) = max(maxes3);
%      % index.(labelP{countP}) = I1(I)
% end

% %cash flow diagram
% for year = 1:18
%     conversionindex = 25;
%     countT = 7;
%     yearlist = ['year' num2str(year)];
%     yearlistprevious = ['year' num2str(year-1)];
%     CumDiscCashFlow(year) = CumulativeDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{countT})(conversionindex);
%     CumCashFlow(year) = CumulativeNonDiscountedCashFlowLoan.(yearlist).(labelP{countP}).(labelT{countT})(conversionindex);
%     CumDiscCashFlowNoLoan(year) = CumulativeDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{countT})(conversionindex);
%     CumCashFlowNoLoan(year) = CumulativeNonDiscountedCashFlowNoLoan.(yearlist).(labelP{countP}).(labelT{countT})(conversionindex);
% end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%-----plotting-----%
countP = 1;
for z=1
%     figure1 = figure('Color',[1 1 1]);
%     figure2 = figure('Color',[1 1 1]);
%     figure3 = figure('Color',[1 1 1]);
figure4 = figure('Color',[1 1 1]);
%     figure5 = figure('Color',[1 1 1]);
%     figure6 = figure('Color',[1 1 1]);
%     figure7 = figure('Color',[1 1 1]);
%     figure8 = figure('Color',[1 1 1]);
figure9 = figure('Color',[1 1 1]);
%     figure10 = figure('Color',[1 1 1]);
figure11 = figure('Color',[1 1 1]);
figure12 = figure('Color',[1 1 1]);
figure13 = figure('Color',[1 1 1]);
figure14 = figure('Color',[1 1 1]);
figure15 = figure('Color',[1 1 1]);
figure16 = figure('Color',[1 1 1]);
%     figure17 = figure('Color',[1 1 1]);

%     figure(figure1)
%     for i = 225:5:240
%         countT = (i - 225)/5 + 1;

```

```

%         hold on
%         % plot mole fraction as function of tau
%         plot(tau.(labelP{countP}).(labelT{countT})).*60,Ethanol.(labelP{countP}).(labelT{countT}), 'Color',cc(countT,:), 'LineWidth',1)
%         xlabel('Residence Time [min]');ylabel('Molar Flow Rate Ethanol [gmol/hr]')
%         %         axis([0 500 4 10])
%         end
%         axes1 = get(figure1,'CurrentAxes');
%         hold(axes1,'on');
%         box(axes1,'on');
%         set(axes1,'FontWeight','bold');
%         %         legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'],...
%         %         ['360' char(176) 'C'], ['380' char(176) 'C'], 'Location','NE','FontSize',11)
%         figure(figure2)
%         for i = 225:5:240
%             countT = (i - 225)/5 + 1;
%             %plot molar flow rate PEtA vs residence time
%             hold on
%             plot((tau.(labelP{countP}).(labelT{countT})).*60,EtA.(labelP{countP}).(labelT{countT}), 'Color',cc(countT,:), 'LineWidth',1)
%             xlabel('Residence Time [min]');ylabel('Molar Flow Rate Ethyl Acetate [gmol/hr]')
%             end
%             %         axis([0 500 0 2.2])
%             axes1 = get(figure2,'CurrentAxes');
%             hold(axes1,'on');
%             box(axes1,'on');
%             set(axes1,'FontWeight','bold');
%             %         legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'],...
%             %         ['360' char(176) 'C'], ['380' char(176) 'C'], 'Location','best','FontSize',11)
%             figure(figure3)
%             for i = 225:5:240
%                 countT = (i - 225)/5 + 1;
%                 %
%                 hold on
%                 plot(xt.(labelP{countP}).(labelT{countT}),sEtA.(labelP{countP}).(labelT{countT}), 'Color',cc(countT,:), 'LineWidth',1)
%                 xlabel('Ethanol Conversion');
%                 ylabel('Ethyl Acetate Selectivity')
%             end
%             %         axis([0 0.6 0.35 0.5])
%             axes1 = get(figure3,'CurrentAxes');
%             hold(axes1,'on');

```

```

%     box(axes1,'on');
%     set(axes1,'FontWeight','bold');
%     %     ylabel = [-30:300]';
%     %     oppoint = 0.25;
%     %     plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%     %     legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176)↵
'C'],...
%     %     ['360' char(176) 'C'], ['380' char(176)↵
'C'],'Location','NE','FontSize',11)
%
%
figure.figure4
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),Revenue.(labelP{countP}).(labelT↵
{countT}),'Color',cc(countT,:),'Marker','sq')
    xlabel('Ethanol Conversion');ylabel('Revenue [MM$]')
end
%     axis([0 0.6 25 40])
axes1 = get(figure4,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%     ylabel = [-30:300]';
%     oppoint = 0.25;
%     plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%     legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'],...
%     ['360' char(176) 'C'], ['380' char(176) 'C'],'Location','Best','FontSize',↵
11)

%
%
figure.figure5
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),Vreal.(labelP{countP}).(labelT↵
{countT})./1000,'Color',cc(countT,:), 'LineWidth',1)
%     xlabel('Ethanol Conversion');
%     ylabel('Reactor Volume [m^3]')
%
end
%     %     axis([0 0.6 0 3*10^3])
%
axes1 = get(figure5,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold');
%     %     ylabel = [-30:30000]';
%     %     oppoint = 0.25;

```

```

%      %      plot(zeros(length(yline),1)+oppoint,✓
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%      %      legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) ✓
'C'],...
%      %      ['360' char(176) 'C'], ['380' char(176) ✓
'C'],'Location','NE','FontSize',11)
%
%      %
%      figure(figure7)
%      for i = 225:5:240
%          countT = (i - 225)/5 + 1;
%          hold on
%          plot(xt.(labelP{countP}).(labelT{countT}), (FEthanol.(labelP{countP}). ✓
(labelT{countT})-PEthanol.(labelP{countP}).(labelT{countT})), 'Color', cc ✓
(countT,:), 'LineWidth',1)
%          xlabel('Ethanol Conversion'); ylabel('Fresh Feed Ethanol [gmol/hr]')
%      end
%      %      axis([0 0.6 160000 240000]);
%      axes1 = get(figure7,'CurrentAxes');
%      hold(axes1,'on');
%      box(axes1,'on');
%      set(axes1,'FontWeight','bold');
%      %      yline = [-30:300]';
%      %      oppoint = 0.25;
%      %      plot(zeros(length(yline),1)+oppoint, ✓
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%      %      legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) ✓
'C'],...
%      %      ['360' char(176) 'C'], ['380' char(176) ✓
'C'],'Location','Best','FontSize',11)
%
%      %
figure(figure9)
for i = 240
    countT = (i - 225)/5 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), NPV.(labelP{countP}).(labelT{ ✓
countT}), 'Color','k', 'LineStyle','none', 'Marker','sq', 'LineWidth',1.5)
    xlabel('Ethanol Conversion')
    ylabel('NPV_{project} [MM$]')
    axis([0.2 0.6 61 65.5])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), NPVpercent.(labelP{countP}).(labelT{ ✓
countT}), 'Color','k', 'LineStyle','none', 'Marker','o', 'LineWidth',1.5)
    ylabel('NPV_%')
    axis([0.2 0.6 5 20])
end

```



```

axes1 = get(figure9, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
yyaxis left
axes1 = get(figure9, 'CurrentAxes');
set(axes1, 'FontWeight', 'bold', 'YColor', 'k');
    yline = [-300:300]';
    oppoint = 0.45;
    plot(zeros(length(yline),1)+oppoint,
yline, 'LineStyle', '--', 'Color', 'k', 'Linewidth',1, 'Marker', 'none')
    %     legend(['340' char(176) 'C'],...
    %           ['360' char(176) 'C'], ['380' char(176) 'C'], 'Location', 'NE', 'FontSize',
11)

%     %
%     figure(figure10)
%     for i = 240
%         countT = (i - 225)/5 + 1;
%         hold on
%         plot(xt.(labelP{countP}).(labelT{countT}), PEther.(labelP{countP}).(labelT{
countT})./PTotal.(labelP{countP}).(labelT{countT}),...
%             xt.(labelP{countP}).(labelT{countT}), PEtA*ones(length(xt.(labelP{
countP}).(labelT{countT})),1)./PTotal.(labelP{countP}).(labelT{countT}),...
%             xt.(labelP{countP}).(labelT{countT}), PEthanol.(labelP{countP}).(
labelT{countT})./PTotal.(labelP{countP}).(labelT{countT}), 'LineWidth',1)
%         yline = [-30:300]';
%         oppoint = 0.25;
%         plot(zeros(length(yline),1)+oppoint,
yline, 'LineStyle', '--', 'Color', 'k', 'Linewidth',1, 'Marker', 'none')
%         legend('x_{Ether}', 'x_{Ethyl Acetate}', 'x_
{Ethanol}', 'Location', 'best', 'FontSize',11)
%         xlabel('Ethanol Conversion');
%         ylabel('Reactor Effluent Mole Fraction')
%     end
%     %     axis([0 0.6 0 1])
%     axes1 = get(figure10, 'CurrentAxes');
%     hold(axes1, 'on');
%     box(axes1, 'on');
%     set(axes1, 'FontWeight', 'bold');

%
figure(figure11)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(NPV.(labelP{countP}).(labelT{countT}), NPVpercent.(labelP{countP}).(labelT{
countT}), 'Color', cc(countT,:), 'marker', 'sq')
end
%     axis([40 80 0 30])

```

```

ylabel('NPV_%')
xlabel('NPV_{project} [MM$]')
axes1 = get(figure11, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
% legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'], ...
% ['360' char(176) 'C'], ['380' char(176) 'C'], 'Location', 'Best', 'FontSize',
11)

%
figure(figure12)
for i = 240
    countT = (i - 225)/5 + 1;
    hold on
    IRRplot.(labelP{countP}).(labelT{countT}) = 100*IRR.(labelP{countP}).(labelT
{countT});
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), IRRplot.(labelP{countP}).(labelT
{countT}), 'Color', 'k', 'Marker', 'sq', 'LineWidth', 1.5, 'LineStyle', 'none')
end
% axis([0 0.6 0 45])
ylabel('IRR [%]')
xlabel('Ethanol Conversion')
axes1 = get(figure12, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
% yline = [-30:300];
% oppoint = 0.25;
% plot(zeros(length(yline), 1) + oppoint,
yline, 'LineStyle', '--', 'Color', 'k', 'Linewidth', 1, 'Marker', 'none')
% legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'], ...
% ['360' char(176) 'C'], ['380' char(176) 'C'], 'Location', 'NE', 'FontSize',
11)

%
figure(figure13)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}), ROI_BT.(labelP{countP}).(labelT
{countT}), 'Color', cc(countT, :), 'Marker', 'sq')
end
% axis([0 0.6 -10 70])
ylabel('ROI_{BT} [%]')
xlabel('Ethanol Conversion')
axes1 = get(figure13, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');

```

```

set(axes1,'FontWeight','bold');
%   yline = [-30:300]';
%   oppoint = 0.25;
%   plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%   legend(['300' char(176) 'C'], ['320' char(176) 'C'], ['340' char(176) 'C'],...
%   ['360' char(176) 'C'], ['380' char(176) 'C'],'Location','NE','FontSize',↵
11)

%
figure(figure14)
for i = 225:5:240
    countT = (i - 225)/5 + 1;
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),TI.(labelP{countP}).(labelT↵
{countT}), 'Color',cc(countT,:), 'Marker', 'sq')
end
%   axis([0 0.6 0 100])
ylabel('TCI [MM$]')
xlabel('Ethanol Conversion')
axes1 = get(figure14, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
%   yline = [-30:300]';
%   oppoint = 0.25;
%   plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')

%
figure(figure15)
for i = 240
    countT = (i - 225)/5 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),ROI_BT.(labelP{countP}).(labelT↵
{countT}), 'Color','k', 'LineStyle','-', 'Marker','sq', 'LineWidth',1)
    xlabel('Ethanol Conversion')
    ylabel('ROI_{BT} [%]')
    %   axis([0 0.6 -10 70])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),TI.(labelP{countP}).(labelT↵
{countT}), 'Color','k', 'LineStyle',':', 'Marker','o', 'LineWidth',1)
    ylabel('TCI [MM $]')
    %   axis([0 0.6 0 100])
end
axes1 = get(figure15, 'CurrentAxes');
hold(axes1, 'on');

```

```

box(axes1,'on');
set(axes1,'FontWeight','bold','YColor','k');
yyaxis left
axes1 = get(figure15,'CurrentAxes');
set(axes1,'FontWeight','bold','YColor','k');
%     ylabel = [-30:300]';
%     oppoint = 0.25;
%     plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
legend(['ROI_{BT}'], ['TI'], 'Location', 'NE', 'FontSize', 11)

%     %
%     figure(figure6)
%     for i = 240
%         countT = (i - 225)/5 + 1;
%         hold on
%         plot(xt.(labelP{countP}).(labelT{countT}), PEther.(labelP{countP}).(labelT↵
{countT})./1000,...
%             xt.(labelP{countP}).(labelT{countT}), PEtA*ones(1,length(xt.(labelP↵
{countP}).(labelT{countT})))./1000,...
%             xt.(labelP{countP}).(labelT{countT}), PEthanol.(labelP{countP}).↵
(labelT{countT})./1000, 'LineWidth', 1.5)
%         hold on
%         plot(xt.(labelP{countP}).(labelT{countT}), FEthanol.(labelP{countP}).↵
(labelT{countT})./1000, 'LineWidth', 1.5)
%         plot(xt.(labelP{countP}).(labelT{countT}), FreshFeed.(labelP{countP}).↵
(labelT{countT})./1000, 'LineWidth', 1.5)
%         %     ylabel = [-30:3000]';
%         %     oppoint = 0.25;
%         %     plot(zeros(length(yline),1)+oppoint,↵
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%         legend('P_{Ether}', 'P_{Ethyl Acetate}', 'R_{Ethanol}', 'F_{Ethanol}', 'F_↵
{Fresh Ethanol}', 'Location', 'best', 'FontSize', 11)
%         xlabel('Toluene Conversion'); ylabel('Molar Flowrate [kgmol/hr]')
%         %     axis([0 0.6 0 10*max(PEtA)./1000])
%         axes1 = get(figure6,'CurrentAxes');
%         hold(axes1,'on');
%         box(axes1,'on');
%         set(axes1,'FontWeight','bold');
%     end
%
%     figure(figure8)
%     %only one temp as PTotal is independent of temp for a given conversion
%     for i = 240
%         countT = (i - 225)/5 + 1;
%         hold on
%         plot(xt.(labelP{countP}).(labelT{countT}), PTotal.(labelP{countP}).(labelT↵
{countT}), 'Color', cc(countT,:), 'LineWidth', 1)
%         xlabel('Ethanol Conversion'); ylabel('Total Flow to Sep Unit [gmol/hr]')
%         %     axis([0 0.6 0 1e7])

```

```

%         axes1 = get(figure8,'CurrentAxes');
%         hold(axes1,'on');
%         box(axes1,'on');
%         set(axes1,'FontWeight','bold');
%         %     ylabel = [-30:300000000]';
%         %     oppoint = 0.25;
%         %     plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%     end
%

%
figure(figure16)
countT = 4;
for j = 2:2:10
    P = j; %bar
    countP = (j-2)/2 + 1;
    yyaxis left
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPV.(labelP{countP}).(labelT↵
{countT}), 'Color',cc(countP,:), 'LineStyle','-', 'Marker','sq', 'LineWidth',1)
    xlabel('Toluene Conversion')
    ylabel('NPV_{project} [MM$]')
    %         axis([0 0.6 -10 80])

    yyaxis right
    hold on
    plot(xt.(labelP{countP}).(labelT{countT}),NPVpercent.(labelP{countP}).(labelT↵
{countT}), 'Color',cc(countP,:), 'LineStyle',':', 'Marker','o', 'LineWidth',1)
    ylabel('NPV_%')
    %         axis([0 0.6 0 30])
end
axes1 = get(figure16,'CurrentAxes');
hold(axes1,'on');
box(axes1,'on');
set(axes1,'FontWeight','bold','YColor','k');
yyaxis left
axes1 = get(figure16,'CurrentAxes');
set(axes1,'FontWeight','bold','YColor','k');
%     ylabel = [-300:300]';
%     oppoint = 0.25;
%     plot(zeros(length(yline),1)+oppoint,↵
ylabel,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%
%     legend(['10 bar'],['20 bar'],...
%         ['30 bar'],'Location','NE','FontSize',11)
%
%
%
%     figure(figure17)

```

```

%     countT = 5;
%     for i = 1:2:5
%         countP = i;
%         hold on
%         plot(xt.(labelP{countP}).(labelT{countT}),Vreal.(labelP{countP}).(labelT{
countT})./1000,'Color',cc(countP,:), 'LineWidth',1)
%         xlabel('Toluene Conversion');
%         ylabel('Reactor Volume [m^3]')
%     end
%     axis([0 0.6 0 1*10^2])
%     axes1 = get(figure17,'CurrentAxes');
%     hold(axes1,'on');
%     box(axes1,'on');
%     set(axes1,'FontWeight','bold');
%     yline = [-30:30000]';
%     oppoint = 0.25;
%     plot(zeros(length(yline),1)+oppoint,
yline,'LineStyle','--','Color','k','Linewidth',1,'Marker','none')
%     legend(['10 bar'],['20 bar'],['30 bar'],'Location','NE','FontSize',11)

```

```
end
```

```

% -----%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

```
% toc
```

```

function F = IRRsolver(rate,p)
countP = p.countP;
countT = p.countT;
labelP = p.labelP;
labelT = p.labelT;
z = p.z;
cashflow = p.cashflow;
NPVIRR.(labelP{countP}).(labelT{countT})(z) = 0;
for year = 1:18
    yearlist = ['year' num2str(year)];
    discount.(yearlist) = (1/((1 + rate)^year));
    NPVIRRCashflow.(yearlist).(labelP{countP}).(labelT{countT}) = cashflow.(yearlist).
(labelP{countP}).(labelT{countT})(z).*discount.(yearlist);
    NPVIRR.(labelP{countP}).(labelT{countT})(z) = NPVIRR.(labelP{countP}).(labelT{
countT})(z) + NPVIRRCashflow.(yearlist).(labelP{countP}).(labelT{countT});
end
F(1) = NPVIRR.(labelP{countP}).(labelT{countT})(z);
end

```

```
function reaction = EtAcetateReactor_PBR_Ideal_184B(V,N,T,P)

%T is in Kelvin
%P is in atm
R = 1.987; %[cal/mol*K]
packingfraction = 0.5*6.31; %g/cm^3 (packing fraction*Cuo density)
%set values for molar flowrates at current step
na = N(1);
nr = N(2);
ns = N(3);
nea = N(4);
ntot = sum(N);
%calc partial pressures at given step
pa = P*na/ntot; %[atm]
pea = P*nea/ntot; %[atm]
ps = P*ns/ntot; %[atm]
%calc equilibrium values
K = exp((-3127/(T))+5.32); %[1/atm]
k = exp((-16310/(R*T))+10.95); %[mol/hr*g-cat]
KA = exp((5890/(R*T))-6.40); %[1/atm]
Kea = exp((11070/(R*T))-9.40); %[1/atm]
KS = exp((6850/(R*T))-7.18); %[1/atm]
%calc reaction rate for ethanol on catalyst
ra = k*KA*((pa^2) - (pea*(ps^2)/K))/((1 + KA*pa + Kea*pea + KS*ps)^2); %[mol/hr*g-cat]
ra = ra*packingfraction; %[mol/hr*cm^3]
ra = ra*1000; %[mol/hr*L]
dH2 = 2*ra;
% dAcetaldehyde = ra;
dEtAcetate = ra;
dEther = (1/10)*ra;
dH2O = dEther;
dAcetaldehyde = 0;
dEthanol = -2*dEtAcetate-2*dEther;

reaction = [dEthanol;dAcetaldehyde;dH2;dEtAcetate;dEther;dH2O];
end
```

```
function NPV = Sensitivity_Hysys_EthylAcetate(Price,EnterpriseRate,InterestRate,✓
IncomeTaxRate,FCImultiplier,SUMultiplier,WCMultiplier)
% %Base Values%%
% Price.Eth = 500;[%$/MT]
% Price.DE = 800;[%$/MT]
% Price.EA = 1100;[%$/MT]
% Price.Fuel = 2.5;[%$/MM BTU]
% Price.CO2 = 40; %$/MT
% Price.Cat = 15000; %$/MT
% EnterpriseRate = 0.1;
% InterestRate = 0.05;
% IncomeTaxRate = 0.27;
% FCImultiplier = 1;
% SUMultiplier = 1;
% WCMultiplier = 1;
% Price.Electricity = 0.08; % $/kw hr

x = 0.45;
EAflow = 50000; %MT/yr
Ethflow = 59514; %MT/yr
DEflow = 3936.24; %MT/yr
Hflow = 4480.56; %MT/yr

MS = 1650;

%heat exchangers
HX1a = 1110; %ft^2
HX2a = 594; %ft^2
HX3a = 2023; %ft^2
HX4a = 1404; %ft^2
HX5a = 116; %ft^2
HX6a = 4; %ft^2
HX1Fc = (0.85+0)*3.75;
HX2Fc = (1.35+0)*3.75;
HX3Fc = (0.85+0)*3.75;
HX4Fc = (0.85+0)*3.75;
HX5Fc = (0.85+0)*3.75;
HX6Fc = (0.85+0)*3.75;

HX1cost = MS/280*101.3*HX1a^(0.65)*(2.29+HX1Fc); %$
HX2cost = MS/280*101.3*HX2a^(0.65)*(2.29+HX2Fc); %$
HX3cost = MS/280*101.3*HX3a^(0.65)*(2.29+HX3Fc); %$
HX4cost = MS/280*101.3*HX4a^(0.65)*(2.29+HX4Fc); %$
HX5cost = MS/280*101.3*HX5a^(0.65)*(2.29+HX5Fc); %$
HX6cost = MS/280*101.3*HX6a^(0.65)*(2.29+HX6Fc); %$

HX2duty = 3.16; %MW
HX3duty = 1.2; %MW
HX4duty = 4.07*3600*8400/1055; %MM BTU/year
HX5duty = 0.76*3600*8400/1055; %MM BTU/year
```



```
HX6duty = 0.01*3600*8400/1055; %MM BTU/year

HX2fuel = HX2duty*1.13; %MW
HX3fuel = HX3duty*1.3; %MW
HX4opcost = HX4duty*Price.Fuel*0.0075*5; %$
HX5opcost = HX5duty*Price.Fuel*0.0075; %$
HX6opcost = HX6duty*Price.Fuel*0.0075; %$

HXcost = sum([HX1cost,HX2cost,HX3cost,HX4cost,HX5cost,HX6cost]);
HXfuelreq = HX2fuel + HX3fuel; %MW
HXopcost = sum([HX4opcost,HX5opcost,HX6opcost]);

%reactor
RD = 1.09*3.28; %ft
RL = 10*3.28; %ft
RFc = 1*3.67;
Rcost = MS/280*101.9*RD^(1.066)*RL^(0.82)*(2.18+RFc); %$
Rduty = 0.585;
Rfuelreq = Rduty*1.13; %MW
RV = (((1.009/2)^2)*pi*10); %m^3
CatMass = RV*6350/1000; %MT

%sep system
%exchangers
D1condHXa = 335*10.7639; %ft^2
D1rebHXa = 260*10.7639; %ft^2
D2condHXa = 51*10.7639; %ft^2
D2rebHXa = 192*10.7639; %ft^2

D1condHXFc = (0.85+0)*3.75;
D1rebHXFc = (0.85+0)*3.75;
D2condHXFc = (0.85+0)*3.75;
D2rebHXFc = (0.85+0)*3.75;

D1condHXcost = MS/280*101.3*D1condHXa^(0.65)*(2.29+D1condHXFc); %$
D1rebHXcost = MS/280*101.3*D1rebHXa^(0.65)*(2.29+D1rebHXFc); %$
D2condHXcost = MS/280*101.3*D2condHXa^(0.65)*(2.29+D2condHXFc); %$
D2rebHXcost = MS/280*101.3*D2rebHXa^(0.65)*(2.29+D2rebHXFc); %$

%operation costs for sep HXers
D1rebHXduty = 9.167; %MW
D2rebHXduty = 5.131; %MW
D1condHXduty = 9.306*3600*8400/1055; %MM BTU/year
D2condHXduty = 4.222*3600*8400/1055; %MM BTU/year

D1rebHXfuel = D1rebHXduty*1.13; %MW
D2rebHXfuel = D2rebHXduty*1.13; %MW

Sepfuelreq = sum([D1rebHXfuel,D2rebHXfuel]); %MW
```

```
D1condHXopcost = D1condHXduty*Price.Fuel*0.0075; %$
D2condHXopcost = D2condHXduty*Price.Fuel*0.0075; %$

%columns
P = 1;
Fm = 3.5;
P0 = 4.5; %bar
t_p = 0.13*(P-P0)./P0;
Fp = 1+t_p*(1+exp(-t_p./2));
Fi = 1.38;
Fd = 3;
Fs = 1; % (for 60 cm tray spacing)
Ft = 0; %sieve
d0 = 1; %m
H0 = 6.1; %m
as = 0.82;
at = 1.8;
Fcshell = (Fm.*Fp -1+Fi.*Fd);
Fctray = (Fs + Ft + Fm);

D1d = mean([2.405,2.625]); %m (avg of stripping and rectifying)
D1H = 13.41+14.63; %m
D1V = (pi*(D1d/2)^2)*D1H;
CostShell = (MS./301).*(Fcshell).*5000.*(D1d./d0)*((D1H./H0).^as); %$
CostTray = (MS./301).*(Fctray).*5000.*((D1d./d0).^at).*(D1H./H0); %$
D1ColCost = CostShell + CostTray; %$

P = 20;
Fm = 3.5;
P0 = 4.5; %bar
t_p = 0.13*(P-P0)./P0;
Fp = 1+t_p*(1+exp(-t_p./2));
Fi = 1.38;
Fd = 3;
Fs = 1; % (for 60 cm tray spacing)
Ft = 0; %sieve
d0 = 1; %m
H0 = 6.1; %m
as = 0.82;
at = 1.8;
Fcshell = (Fm.*Fp -1+Fi.*Fd);
Fctray = (Fs + Ft + Fm);

D2d = mean([3.464,3.561]); %m (avg of stripping and rectifying)
D2H = 17.07+16.46; %m
D2V = (pi*(D2d/2)^2)*D2H;
CostShell = (MS./301).*(Fcshell).*5000.*(D2d./d0)*((D2H./H0).^as); %$
CostTray = (MS./301).*(Fctray).*5000.*((D2d./d0).^at).*(D2H./H0); %$
D2ColCost = CostShell + CostTray; %$
```

```

Sepcost = sum([D1condHXcost,D1rebHXcost,D2condHXcost,D2rebHXcost,...
    D1ColCost,D2ColCost]);
SepOpcost = sum([D1condHXopcost,D2condHXopcost]);

Fuel = (HXfuelreq+Sepfuelreq+Rfuelreq)*3600*8400/1055; %MM BTU/yr
FuelRefund = (DEflow*2726.3*74.123/1e6 + Hflow*286*2.016/1e6); %kJ/year
FuelRefund = 0.7*FuelRefund/1055000; %MM BTU/yr
% Fuel = Fuel-FuelRefund;
CO2prod = 4*(DEflow/74.123)*44.01; %MT/yr
CO2perMassProd = CO2prod/EAflow; %kg/kg

%fixed Costs
ISBL = Sepcost + Rcost + HXcost + 160000 + 100000; %$
FCI = 2.28*ISBL; %$
FCI = FCI*FCImultiplier;
SU = 0.1*FCI; %$
SU = SU*SUmultiplier;

Salvage = 0.01*FCI; %$
WC = Ethflow*Price.Eth*1/12; %$/yr
WC = WC*Wcmultiplier;

TI = FCI + SU + WC; %$
FuelCost = Price.Fuel*Fuel; %$/yr
OPEX = FuelCost + SepOpcost + HXopcost + 70000 + 20000; %$
Revenue = EAflow*Price.EA; %$/yr
AGS = 0.1*Revenue; %$
ReactantCost = Ethflow*Price.Eth; %$/yr
CatalystCost = CatMass*Price.Cat; %$/yr
ConstructionLoan = FCI + WC + SU; %$
CO2cost = CO2prod*Price.CO2; %$/yr
COM = OPEX + AGS + CO2cost + ReactantCost; %$
FCneg3 = -0*FCI;
FCneg2 = -0*FCI;
FCneg1 = -0.6*FCI;
FC0 = -0.4*FCI;
WC0 = -WC;
SU0 = -SU;

FCneg3disc = (1/(1+InterestRate)^(-3))*FCneg3;
FCneg2disc = (1/(1+InterestRate)^(-2))*FCneg2;
FCneg1disc = (1/(1+InterestRate)^(-1))*FCneg1;
FC0disc = FC0;
WC0disc = WC0;
SU0disc = SU0;

BondPrinciple = sum([FCneg3disc,FCneg2disc,FCneg1disc,FC0disc,WC0disc,SU0disc]);

```

```
BondInterestPayments = BondPrinciple*(InterestRate-0.02);

ProfitBeforeTax = Revenue - COM;
Depreciation = (FCI + SU - Salvage)/10; %$/yr

for i = 1:15
    if i == 1
        Productivity = 0.5;
    else
        Productivity = 1;
    end

    CatYear = 1;

    if i<=10
        DepYear = 1;
    else
        DepYear = 0;
    end
    BondFinancing(i) = BondInterestPayments*DepYear;
    ProfitBT(i) = Productivity*ProfitBeforeTax - CatalystCost*CatalystCost*CatYear*2 + BondFinancing(i);
    DepreciationAllowed(i) = Depreciation*DepYear;
    ProfitAfterTaxes(i) = (ProfitBT(i) - ...
        DepreciationAllowed(i))*(1-IncomeTaxRate);
    cashflow(i) = ProfitAfterTaxes(i) + DepreciationAllowed(i);

end

cashflow(10) = cashflow(10) + BondPrinciple + ((ProfitBT(i) - ...
    DepreciationAllowed(i))*(IncomeTaxRate));
cashflow(15) = cashflow(15) + WC + Salvage;
for i = 1:15
    disccashflow(i) = (1/(1+EnterpriseRate)^i)*cashflow(i);
end

NPV0 = sum(disccashflow);
NPVproject = NPV0*(1+EnterpriseRate)^(-2); %$
NPV = NPVproject/1e6;

end
```

```
clear
close all
N = 10000;
tic
NPVlist = zeros(1,N);
for k = 1:N
    % tic
    %range of effects [-%, +%]
    EnterpriseRate = 0.1;
    GeneralRange = [-.1 .1];

    EthRange = [-0.01 0.01];
    DERange = [-.25 .5];
    EARange = [-.32 .24];
    FuelRange = GeneralRange;
    CO2Range = GeneralRange;
    CatalystRange = GeneralRange;
    InterestRateRange = [-.5 .5];
    IncomeTaxRateRange = [-.5 .5];
    FCIRange = [-.1 .25];
    SURange = [-.1 1.0];
    WCRRange = [-.2 .5];

    Price.Eth = 500; %[$/MT]
    Price.DE = 800; %[$/MT]
    Price.EA = 1200; %[$/MT]
    Price.Fuel = 2.5; %[$/MM BTU]
    Price.CO2 = 40; %$/MT
    Price.Cat = 10000; %$/MT
    InterestRate = 0.05;
    IncomeTaxRate = 0.27;
    FCImultiplier = 1;
    SUMultiplier = 1;
    WCMultiplier = 1;

    M(1,1) = Price.Eth;
    M(1,2) = Price.DE;
    M(1,3) = Price.EA;
    M(1,4) = Price.Fuel;
    M(1,5) = Price.CO2;
    M(1,6) = Price.Cat;
    M(1,7) = InterestRate;
    M(1,8) = IncomeTaxRate;
    M(1,9) = FCImultiplier;
    M(1,10) = SUMultiplier;
    M(1,11) = WCMultiplier;

    M([2 3],1) = EthRange;
    M([2 3],2) = DERange;
    M([2 3],3) = EARange;
```

```

M([2 3],4) = FuelRange;
M([2 3],5) = CO2Range;
M([2 3],6) = CatalystRange;
M([2 3],7) = InterestRateRange;
M([2 3],8) = IncomeTaxRateRange;
M([2 3],9) = FCIRange;
M([2 3],10) = SURange;
M([2 3],11) = WCRRange;
L = length(M(1,:));
%assume triangle distributions for all ranges
for q = 1:L
    % lower bound
    a(q) = (1+M(2,q))*M(1,q);
    % base value
    b(q) = M(1,q);
    % upper bound
    c(q) = (1+M(3,q))*M(1,q);
    pd = makedist('Triangular','a',a(q),'b',b(q),'c',c(q));
    M(4,q) = random(pd,1);
end

Price.Eth = M(4,1);%[$/MT]
Price.DE = M(4,2);%[$/MT]
Price.EA = M(4,3);%[$/MT]
Price.Fuel = M(4,4);%[$/MM BTU]
Price.CO2 = M(4,5); %$/MT
Price.Cat = M(4,6); %$/MT
InterestRate = M(4,7);
IncomeTaxRate = M(4,8);
FCImultiplier = M(4,9);
SUMultiplier = M(4,10);
WCMultiplier = M(4,11);

NPV = Sensitivity_Hysys_EthylAcetate(Price,EnterpriseRate,InterestRate,...
    IncomeTaxRate,FCImultiplier,SUMultiplier,WCMultiplier);
NPVlist(k) = NPV;
end

% make cdf of NPVlist
orderedNPVlist = sort(NPVlist);
prob = zeros(length(orderedNPVlist),1);
for z = 1:length(orderedNPVlist)
    prob(z) = (z-1)/length(orderedNPVlist);
end

%plot histogram
figure1 = figure('Color',[1 1 1]);
histogram(NPVlist,'Normalization','probability','FaceColor',[0.5 0.5 0.5],'FaceAlpha',.✓
3)

```

```
ylabel('\boldmath{$Probability$}','Interpreter','latex','FontSize',12);
xlabel('\boldmath{$NPV, [MM\$\$}','Interpreter','latex','FontSize',12);
axes1 = get(figure1, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');

%plot cdf
figure1 = figure('Color',[1 1 1]);
plot(orderedNPVlist,prob,'Marker','s','Color','k','LineStyle','none','LineWidth',1)
ylabel('\boldmath{$Probability$}','Interpreter','latex','FontSize',12);
xlabel('\boldmath{$NPV_{project}$}','Interpreter','latex','FontSize',12);
axes1 = get(figure1, 'CurrentAxes');
hold(axes1, 'on');
box(axes1, 'on');
set(axes1, 'FontWeight', 'bold');
% toc
```