

**TECHNO-ECONOMICS AND LIFE CYCLE ANALYSIS OF UPGRADING  
WOODY BIOMASS TO DIESEL BLENDSTOCK**

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## THESIS ACCEPTANCE STATEMENT

On behalf of the Graduate Committee for Aysan Najd Mazhar I affirm that this manuscript is the final and accepted thesis. Signatures of all committee members are on file with the Graduate School at the University of Maine, 5775 Stodder Hall, Orono Maine.

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# **TECHNO-ECONOMICS AND LIFE CYCLE ANALYSIS OF UPGRADING WOODY BIOMASS TO DIESEL BLENDSTOCK**

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Thesis Advisor: Dr. Clayton Wheeler

An Abstract of the Thesis Presented  
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Woody biomass conversion to transportation fuels have been developed as alternatives to fossil fuel production to reduce greenhouse gas emissions and to increase energy security. Fast pyrolysis, a thermochemical technology, has the potential to offer high efficiencies to produce liquid transportation fuels from woody biomass. Fast pyrolysis involves rapid heating of biomass particles in the absence of air at approximately 500°C and results in non-condensable gases, bio-oil (pyrolysis oil), and char as products. The pyrolysis oil can be upgraded via integrated mild hydrogenation and etherification processes to a high energy density fuel that can be blended with diesel for transportation use.

A techno-economic analysis (TEA) and a life cycle analysis (LCA) have been conducted for producing a renewable diesel blendstock by fast pyrolysis and etherification over a mild hydrogenation process as an upgrading pathway. A process simulation was created using Aspen Plus<sup>®</sup> and for the base case simulations, the fast pyrolysis temperature of 500 °C was assumed. Thermodynamic properties of the hydrogenation and etherification model compounds were estimated using Density Functional Theory (DFT). The feedstock and product compositions and yields for pyrolysis were selected from published literature. The results from the process simulation were used to estimate the capital and operating costs for a plant with a capacity factor of 0.9 and process scale of 2,000 dry metric tons per day of forest residues. For the TEA cash flow, we used the economic assumptions and methodologies in the NREL/PNNL report by Dutta, 2015. Dutta's capital costs (updated to 2019 U.S. dollars) and operating costs were used wherever appropriate, and new equipment costs were estimated using correlations from Turton, 2012. The discounted cash flow analysis with an internal rate of return of 10% was selected to assess the minimum fuel selling price (MFSP) of diesel fuel blendstock. The well-to-wheel LCA has been conducted using Argonne's GREET 2019 software to assess environmental sustainability for producing renewable diesel fuel blendstock.

The assessed MFSP of renewable diesel fuel blendstock for the base case is \$2.99 per diesel gallon equivalent (DGE). The results of the fast pyrolysis temperature effect on the MFSP of diesel fuel blendstock have shown that the MFSP can be reduced to \$2.74 per DGE when the fast pyrolysis temperature is decreased to 480 °C. Such a reduction in MFSP is due to the enriched composition of phenols and furans in pyrolysis oils produced at 480 °C. The LCA well-to-wheels

analysis indicates that the renewable diesel blendstock would have a 93% reduction in fossil fuel use and a 93% reduction in greenhouse gas emissions relative to petroleum diesel.

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## **LIST OF ABBREVIATIONS AND DEFINITIONS**

1 metric ton = 1000 kg

mm: millimeter

ASPEN: Advanced Simulator for Process Engineering (Software)

ANN: Artificial Neural Network

CEPCI: Chemical Engineering Plant Cost Index.

DGE: Diesel Gallon Equivalent

EIA: Energy Information Administration

FAME: Fatty Acid Methyl Ester

GHG: Greenhouse Gas Emissions

HMF : Hydroxy Methyl Furfural

IRR: Internal Rate of Return

ISBL: Inside Battery Life; Inner costs of a plant

LCA: Life Cycle Analysis

MM: Million

MFSP: Minimum Fuel Selling Price

MTPD: Metric Tonnes Per Day

NCG: Non-condensable Gases

NREL: National Renewable Energy Laboratory

PNNL: Pacific Northwest National Laboratory

TCI: Total Capital Costs

TIC: Total Installed Costs

TDC: Total Direct Costs

TEA: Techno-economic Analysis

## **CHAPTER 1: INTRODUCTION**

### **1.1 Environmental Impacts of the Petroleum-based Fuels Emissions**

Fossil fuels are the principal supplier of almost all of the world's transportation fuels. The transportation sector is heavily dependent on conventional hydrocarbon fuels such as gasoline and diesel fuels [1]. The incomplete combustion of gasoline and diesel results in emissions of unburned hydrocarbons (HC), carbon monoxide (CO), nitrogen oxides (NO<sub>x</sub>), and soot [2]. More specifically, NO<sub>x</sub> and soot have the highest proportion of diesel emissions [3]. CO, NO<sub>x</sub>, and soot have a significant impact on human health and the environment [4]. For instance, the chemical reactions between nitrogen oxides (NO<sub>x</sub>) and volatile organic compounds contribute to creating tropospheric or ground-level ozone in the presence of heat and sunlight. Getting exposed to ozone can destructively affect sensitive vegetation and ecosystems such as forests and wilderness areas [5]. The inhalation of soot particles may result in important long-term health issues such as asthma and lung cancer. [3]

Crude oil exploration, extraction and processing to transportation fuels (gasoline, jet, and diesel), and combustion of these fuels emit greenhouse gas emissions (e.g., CO<sub>2</sub>). In 2019 the U.S. Energy Information Administration (EIA) estimated that the transportation sector contributes to the emission of 456 million metric tons of carbon dioxide (CO<sub>2</sub>) through diesel fuel consumption which is equal to 24% of the total U.S. transportation sector and 9% of total U.S. energy-related CO<sub>2</sub> emissions [6]. Figure 1 shows that the carbon dioxide emissions in the United States have increased 3 % from 1990 to 2019 [7].

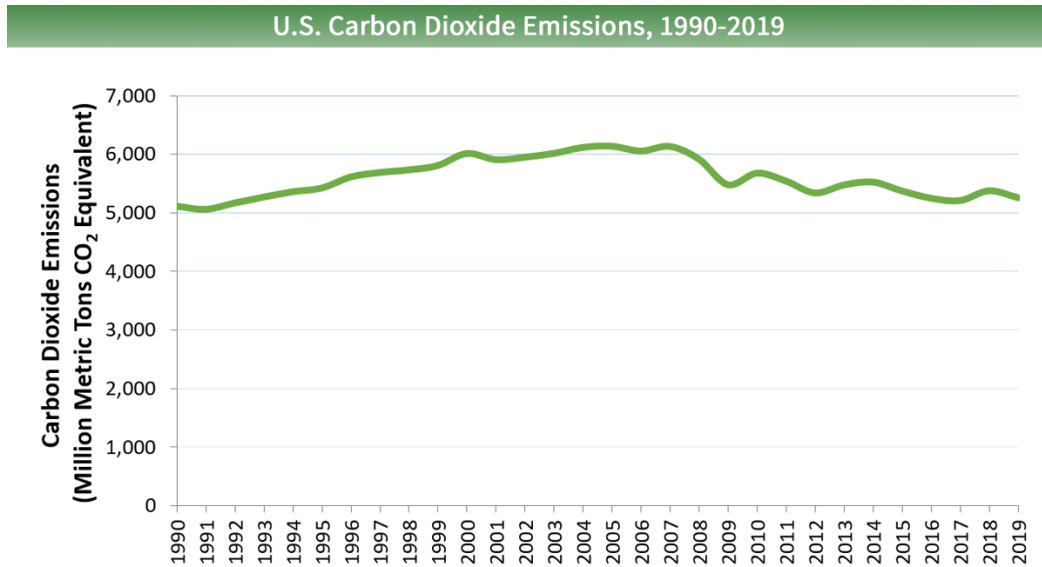


Figure 1. Carbon Dioxide Emissions in the U.S., 1990-2019. Source: epa.gov

## 1.2 Alternative Oxygenated Fuels

Oxygenated fuels (alcohols, ethers, acetals, esters) have been investigated as a promising alternative to conventional fuel in internal combustion engines by providing high thermal efficiency and lower soot emissions. Further, the production of oxygenated fuels from renewable biomass (e.g., wood chips, corn stover, etc.) may have the potential to reduce greenhouse gas emissions when compared to the production of fossil fuels. The oxygenated fuels either can be used as a diesel blendstock or can be used as a diesel substitute. For instance, corn derived ethanol is currently blended with gasoline up to 10% (by volume) in the U.S. Fatty acid methyl esters (FAME) made from fats and vegetable oils and biomass-derived oxymethylene ethers have the potential to substitute for petroleum-derived diesels. Though there is little success with the introduction of diesel substitutes to the market, there is a huge potential for new oxygenated fuels with a potential ranging from diesel blendstock to diesel substitute.



The oxygenated fuels derived from a renewable feedstock (e.g., wood chips and corn stover) via thermochemical technologies (e.g., pyrolysis) usually result in a mixture of a wide range of compounds with varying chemical functionality. For instance, fast pyrolysis oil derived from a lignocellulosic feedstock is a complex mixture of oxygenated compounds. The complex fuel mixtures with a range of oxygenated compounds may not perform optimally when used in internal combustion engines because some of the oxygenated compounds are non-volatile. In other words, the cetane number of the fuel mixtures with a range of oxygenated compounds is much less than the desired minimum cetane number of 40. The cetane number of the complex fuel mixtures (such as pyrolysis oil) can be improved via catalytic transformation of complex oxygenated molecules to simple oxygenated intermediates. The development of such chemical transformation pathways and target oxygenated intermediates in the upgraded fuel can be guided with predictive modeling [8]. For instance, Hunter et al. [8] used existing data sets (fuel molecules and corresponding cetane number) to train algorithms based on artificial neural networks and deduce the structure (chemical functionality) and property (cetane number) relations. Further Hunter et al. [8] use this algorithm to determine the properties (like cetane number, research octane number, and yield sooting index, etc.) of diesel fuel blended with oxygenated fuels.

### **1.3 Fast Pyrolysis Process**

Fast pyrolysis process has attracted interest for converting woody biomass into liquid fuels containing a wide range of oxygenates due to its simplicity, low emissions, scale-up flexibility, high bio-oil yield, and economic efficiency [9].

In the fast pyrolysis process, biomass conversion occurs at a very high heating rate and very short residence time in the absence of oxygen. Pyrolysis oil has yields ranging from 65% to 80% on a dry biomass basis. The byproducts of the fast pyrolysis reaction are bio-char and non-condensable gases (NCGs) [10]. Biomass feedstock properties (e.g., particle size and moisture content) and pyrolysis operating conditions (e.g., temperature and residence time) affect the yields of bio-oil, char, and NCGs.

The optimal conditions to maximize the bio-oil yields and minimize the total energy consumption of the pyrolysis process are fast pyrolysis temperature of between 450-550°C, biomass particle size of 2 mm [11], biomass moisture content of 10 wt.% [12].

### **1.4 Bio-oil Composition and Characteristics**

Pyrolysis oil is a complex mixture of hundreds of organic compounds (hydrocarbons, organic acids, ketones, aldehydes, and phenols). Many factors such as feedstock type and reaction conditions affect the composition of bio-oil. The low heating value, poor thermal and chemical stability, low pH values (high acidity), high viscosity, and a high corrosiveness of pyrolysis oils is due to the low hydrogen content (5-7 weight %) together with a very high oxygen content (about 30-45 wt.%) of pyrolysis oils. Moreover, the high oxygen content of the bio-oil makes it

chemically unstable due to the polymerization reactions occurring between oxygenates [13]. The oxygen content of the pyrolysis oils can be reduced via a number of upgrading pathways like hydrotreating and esterification.

### **1.5 Bio-oil Upgrading Approaches and Challenges**

The hydrotreating of bio-oils to hydrocarbon fuels has been extensively investigated. In the hydrotreating process, pyrolysis oil is contacted with excess hydrogen in presence of suitable catalysts and reaction conditions to produce gas and two liquid fractions. The gas phase contains light hydrocarbons and carbon dioxide. One liquid fraction predominantly contains water and the other liquid fraction contains hydrocarbons, which separate easily. The extent of oxygen removal from biomass and the yields of hydrocarbon fuel is dependent on the catalyst, reactor configuration, and reactor operating conditions. Rapid catalyst deactivation during hydrotreating, severe hydrotreating operating conditions, high hydrogen demand, and the need of at least three reactor steps (hydrogenation, hydrodeoxygenation, and hydrocracking) result in high capital and operating costs of complete hydrodeoxygenation of pyrolysis oils. Further, the high hydrogen demand increases the non-renewability of the hydrotreating process.

A moderate removal of the oxygen content of pyrolysis oils while still being able to use resulting pyrolysis oil as a diesel blendstock can overcome the challenges of hydrotreating pyrolysis oils to hydrocarbons. Mild upgrading process conditions together with providing the hydrogen demand of upgrading process using bio-oil off-gas can result in overcoming the hydrotreating challenges.

Esterification is a reaction between an alcohol and an organic acid in presence of an acid catalyst to form esters. Sondakh et al. [14] studied the bio-oil characteristic improvement via the esterification approach. They evaluated the effect of two acid catalysts ( $\text{H}_2\text{SO}_4$  and  $\text{HCl}$ ) on bio-oil quality enhancement. It has been reported that the chemical reactions between ethanol/methanol and organic acids of the bio-oil in the esterification process lead to reducing viscosity and acidity while increasing the heating value of the pyrolysis oil. The use of acid catalysts showed high esterification activity, which increased the heating value of bio-oils from 13.12 to 20.17 MJ/kg and reduced the water and ash content from 25 wt % to 0.83 wt. % and 0.02 to 0.0003 wt. %, respectively [14].

The dehydration of pyrolysis oils to a high energy density fuel (an upgrading pathway) for use as a diesel blendstock has currently been investigated at the University of Maine. More specifically, the focus is on etherification reactions to convert aromatic alcohols of pyrolysis oil into ethers. The dehydration reactions contribute to stabilizing pyrolysis oil by taking alcohol groups and creating ether groups which are much less reactive and can provide oxygen for cleaner-burning of diesel fuels. A mild hydrogenation step is required before etherification reactions to ensure that all bonds are fully saturated to make the etherification products useful in fuel applications. To facilitate these reactions, solid acid catalysts were used. Solid catalysts relative to homogeneous catalysts have been shown to simplify downstream processing since they can be retrieved with physical separation processes, allowing easier product purification. The model reactants for etherification were tetrahydrofurfuryl alcohol (THFA) and 2-methyl cyclohexanol (2MCH). The research is in progress with the next steps to conduct etherification reactions over solid acid catalyst followed by hydrogenation reactions over Pd/C with pyrolysis oil that has been supplied by the collaborators from UMass Lowell.

## **1.6 Techno-economic Analysis and Life Cycle Assessment**

The techno-economic analysis (TEA) and the life cycle assessment (LCA) methodologies have widely been used to assess the economic viability and environmental sustainability of biomass conversion pathways to fuels, respectively. In simplest terms both TEA and LCA involve simulating a process model of converting biomass to a fuel blendstock using process simulation software like Aspen. The simulated material and energy balances are inputted to a LCA software such as GREET to assess the environmental sustainability of biomass conversion technologies in terms of mid-point environmental impact categories like global warming potential and non-renewable energy use. The Greenhouse, Regulated Emissions and Energy in Transportation (GREET) [15] model is an standard analytical tool in performing life cycle analysis developed by Argonne National Laboratory simulates the energy use and emissions of different vehicles and fuels and sponsored by Department of Energy's office of Energy efficiency and Renewable Energy. This software includes a wide range of feedstocks, fuels and vehicles and fuel pathways including petroleum fuels, biofuels, electricity produced from different feedstock resources. To simulate the biomass conversion to transportation fuel pathway, type and amount of feedstock, energy imported to the process (e.g., electricity, natural gas) and products and energy that have been produced are inputted to the simulated pathway. Based on the existing data sets in GREET (e.g., resources, pollutants, vehicles, transportation modes) and inputted information, this model calculates total energy consumption, emissions of greenhouse gases and air pollutants of the simulated process.

In TEA, the simulated material and energy balances are used as a basis to assess the capital and annual operating costs of biomass conversion pathways. Further, the discounted cash flow methodology will be employed to assess the minimum fuel selling price (MFSP). A wide range of TEA and LCA studies have been conducted to assess the economic viability and environmental sustainability of integrated fast pyrolysis and upgrading pathways to hydrocarbon fuels from lignocellulosic feedstock [[9],[16]]. Table 1 shows the previous TEA and LCA results of biomass derived pyrolysis oil and upgrading processes. Biomass type and composition and upgrading process conditions and steps significantly affect the MFSP of the final product. The TEA analysis has shown that it is possible to produce hydrocarbon fuels from lignocellulosic feedstock at a MFSP of less than \$3.00 per gallon. However, technological challenges like deactivation of hydrotreating catalyst must be overcome to realize such cost targets. The LCA studies have indicated that about 75% of greenhouse reduction is possible with the replacement of crude oil-derived transportation fuels with biomass-derived transportation fuels via a fast pyrolysis pathway.

Table 1. Previous TEA and LCA Studies of Biomass Conversion to Transportation Fuels

Parameters	Brown et. al [17]	Dutta et. al [16]	PNNL [18]
Facility size (dry ton per day)	2000	2000	2000
Feedstock	Corn stover	50% forest residues/ 50% clean pine	50% logging residues /50% forest thinings
Feedstock price(\$/ton)	83(dry ton)	67(dry ton)	30 (50% moisture)
Pyrolysis oil yields(dry basis)	63 wt. %	64 wt. %	51.2 wt. %
Upgrading pathway	Mildhydrotreating /Hydrocracking	Hydrotreating /Hydrocracking	Hydrotreating /Hydrocracking
Upgrading Catalyst	CoMo	Pt/TiO <sub>2</sub>	NiMo
Hydrogen source	Merchant (\$1.33/kg)	Co-hydroprocessing Steam-reforming of natural gas	Onsite – steam reforming of offgas
Total Capital Investment (TCI)	429 \$MM	544 \$MM	358 \$MM
IRR	10%	10%	10%
Product	Renewable diesel	Diesel blendstock	Diesel/Gasolin
MFSP	\$2.57/gal	\$3.12/gal	\$3.09/gal
GHG reduction	53%	78%	63%

In this research, TEA and LCA have been performed to assess the economic viability and environmental sustainability of the production of a renewable diesel blendstock from pine sawdust via integrated fast pyrolysis, mild hydrogenation, and etherification processes, respectively. The Aspen Plus<sup>®</sup> simulation software was used to simulate the conversion process of biomass into fuel blendstock and determine material and energy balances. The results from the process simulation were used to estimate the capital and operating costs for a plant with a capacity factor of 0.9 and processing 2,000 dry metric tons per day of forest residues. The discounted cash flow analysis with an internal rate of return of 10% was selected to assess the MFSP of diesel fuel blendstock. The sensitivity of pyrolysis operating conditions to the fuel blendstock MFSP was measured. The well-to-wheel LCA has been conducted using Argonne's GREET 2019 software to assess environmental sustainability for producing renewable diesel fuel blendstock.



## CHAPTER 2: PROCESS DESCRIPTION

Figure 2 represents a process flow diagram for the pine sawdust conversion into renewable transportation fuel blendstock via integrated fast pyrolysis, hydrogenation, and etherification processes. The pine sawdust is ground to attain a particle diameter of 2 mm, which is followed by drying to reduce the moisture content of pine sawdust to 10 wt. % from 40 wt.%. The composition of pine sawdust used in the simulation is shown in Table 2. It has been reported that biomass ash content is one of the catalyst deactivation contributors during fast pyrolysis reactions [19]. Thus, the amount of ash in the feedstock is one of the important factors in the pyrolysis reaction.

Table 2. Ultimate Analysis of Pine Sawdust Feedstock

Component	Weight % (dry basis)
C	51.42
H	6.04
O	42.43
N	0.09
S	0.02
Ash	0.29
HHV [MJ/kg]	18.98
Heat capacity [Cal /g *K]	0.33

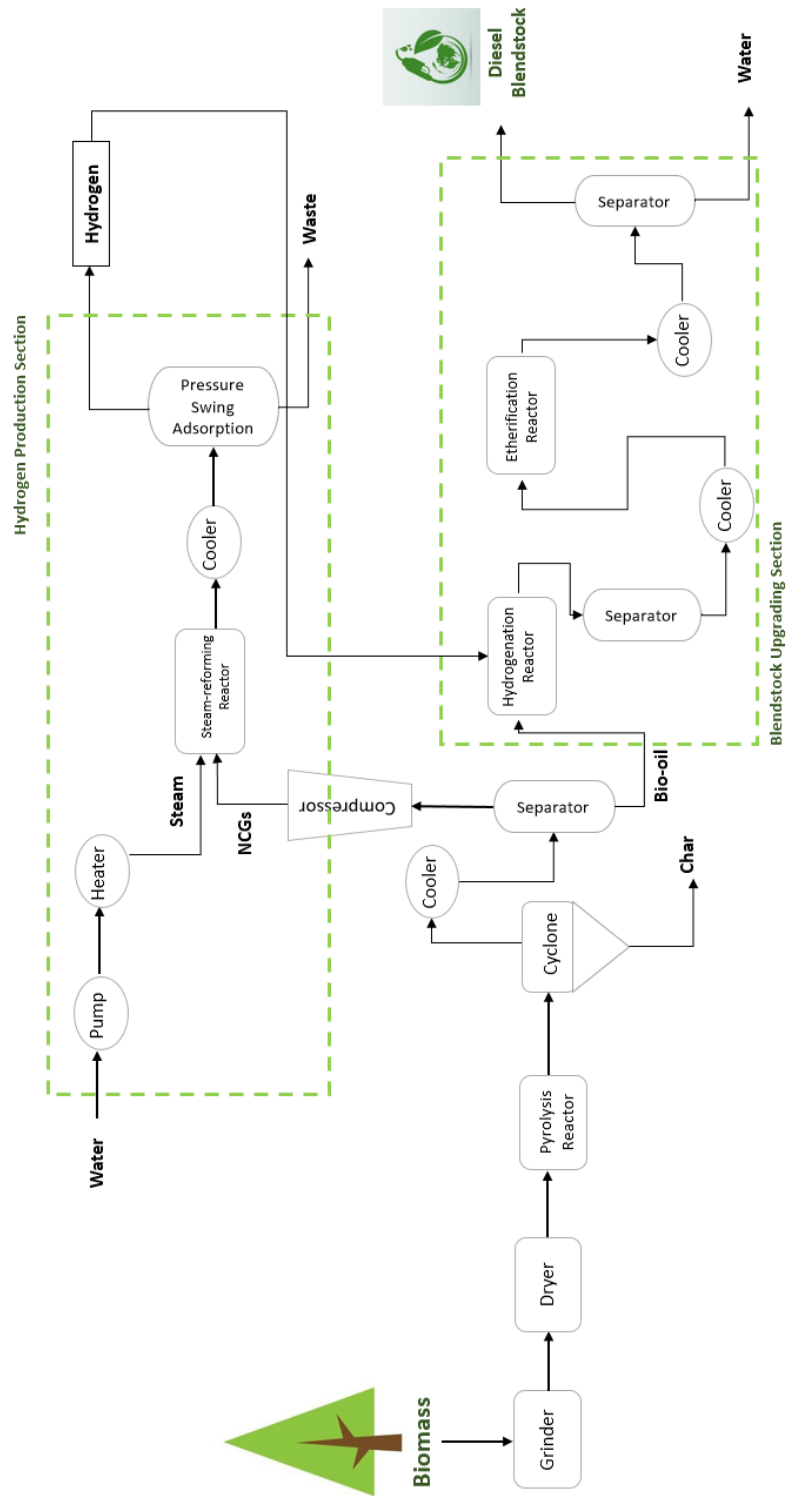


Figure 2. Process Flow Diagram

The dried sawdust is sent to a pyrolysis reactor operating at 500°C. Under fast pyrolysis conditions, pine sawdust depolymerizes to char, non-condensable gases (NCG), and an oil that is a mixture of hundreds of organic compounds. The pyrolysis products are then sent to a cyclone to separate char from the remaining products. The remaining products were cooled down to 25°C and then a separator is used to collect condensable vapors as pyrolysis liquid oil and the NCGs are collected as vapor. The liquid pyrolysis oil upgrading section includes two processes: mild hydrogenation and etherification. The pyrolysis oil is very unstable due to the presence of reactive compounds and thus mild hydrogenation of pyrolysis oil was done before etherification reaction to stabilize pyrolysis oil. Hydrogenation is done under mild conditions of 180 °C and 17 bar in a fixed-bed jacketed reactor in presence of (Pd/C) catalyst [17]. Hydrogen for the hydrogenation process is derived via steam reforming of NCGs. A separator is used to remove the residual hydrogen from the hydrogenated oil and then a heat exchanger is used to cool down the stream to the 118°C temperature to enter the etherification reactor. The etherification reactor is operated at 160 °C and 4 bar in presence of an acid catalyst (BEA-zeolite). The etherified oil then is cooled down to 25°C. Finally, water formed during the etherification process is decanted to collect a high-quality bio-oil.

## **CHAPTER 3: PROCESS SIMULATION**

The Aspen Plus<sup>®</sup> software was employed to simulate the material and energy balance of a biomass conversion pathway shown in Figure 2. The processing capacity of 2000 dry metric tons of sawdust was assumed. The pine sawdust was defined in ASPEN using the ultimate analysis shown in Table 2. The pine sawdust, char, and ash were modeled as nonconventional solid components in Aspen Plus<sup>®</sup>. The general coal enthalpy model (HCOALGEN) was used to calculate the properties of non-conventional compounds. In this model, the user input value option was selected for the heat of combustion (HCOMB). The heat of combustion of wood and char were assumed as 18.98 (MJ/kg) and 31.6 (MJ/kg), respectively. The Boie correlation was selected to assess the heat of the combustion of ash. The standard heat of formation of all nonconventional compounds was calculated using the heat of combustion-based correction, which requires imputing the data of ultimate, proximate, and sulfur analysis of nonconventional compounds. The heat capacities of all non-conventional compounds were assessed using the cubic temperature equation (Kirov correlation). Finally, the enthalpy of nonconventional compounds was calculated based on the heat of combustion.

### **3.1 Pyrolysis Process Simulation**

The pyrolysis mass yields for the base case scenario (which is operating pyrolysis at 500 °C) were assumed at 53.2% bio-oil, 12% char, 23.1 % NCGs, and 11.7% water which are represented in Table 3. The elemental composition of pyrolysis oil organics and char as well as the chemical composition of NCGs used in the simulations are presented in Tables 4 and 5 (personal communication from University of Massachusetts).

Table 3. Pyrolysis Yields (Base-case)

<b>Pyrolysis yields</b>	<b>wt. %</b>
<b>Pyrolysis oil (water-free)</b>	53.2
<b>Char</b>	12
<b>NCG</b>	23.1
<b>Water</b>	11.7

Table 4. Elemental Analysis and HHV of the Pyrolysis Products

<b>Element</b>	<b>Organic wt. %</b> (water-free basis)	<b>Char wt. %</b>
<b>C</b>	54.017	82.7
<b>H</b>	6.3471	3.31
<b>O</b>	39.045	12.16
<b>N</b>	0.5706	1.79
<b>S</b>	0.02	0.04
<b>Ash</b>	0	20.4
<b>HHV [MJ/kg]</b> (Dry ash-free basis)	20	29.7

Table 5. Non-condensable Gases Chemical Composition

<b>NCG</b>	<b>Mol %</b>
<b>CO</b>	40.561
<b>CO<sub>2</sub></b>	35.077
<b>CH<sub>4</sub></b>	12.194
<b>C<sub>2</sub>H<sub>4</sub></b>	0.52
<b>H<sub>2</sub></b>	11.648

To model the bio-oil in the Aspen Plus<sup>®</sup> simulation, model compounds consisting of the ones which are generally known to exist in pyrolysis oil [18] and also in Aspen data banks were selected. The composition of the selected bio-oil compounds was assessed using the experimentally determined elemental (CHO) composition and lower heating values of bio-oil.

A minimization function is applied to determine the mass fraction of the selected compounds. This function takes the elemental analysis results of the pyrolysis oil and computes the mass fractions of the model compounds which governs having a mixture with elemental composition and energy amount parallel to bio-oil. The stoichiometric coefficients of the compounds were determined by using constraints for compositions based on Lyu, et al. [20] and applying the residual error method in Mathcad. These selected small subsets of model compounds including acids, phenols, furans, sugars, ketones, and alcohols which greatly affect the pyrolysis and upgrading processes. A list of the selected model compounds and their stoichiometric coefficients are presented in Table 6.

Table 6. Aspen Plus<sup>®</sup> Model Compounds to Represent Bio-oil

Compound		CAS Number	Stoichiometric Coefficients
Acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	64-19-7	0.097
Phenol	C <sub>6</sub> H <sub>6</sub> O	108-95-2	0.141
HMF	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	67-47-0	0.0452
Levoglucosan	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>	498-07-7	0.0656
Hydroxyacetone	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	116-09-6	0.167
Hydroquinone	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	123-31-9	0.0483

### 3.2 Simulation of Pyrolysis Oil Upgrading

The reaction schemes used to model hydrogenation and etherification reactions are shown in Figures 3 and 4. All the selected model compounds for bio-oil upgrading products except cyclohexanol, are not available in the Aspen database. Therefore, thermodynamic properties of these compounds were estimated using density functional theory (DFT) and imported to Aspen Plus<sup>®</sup> simulation as user-defined components.

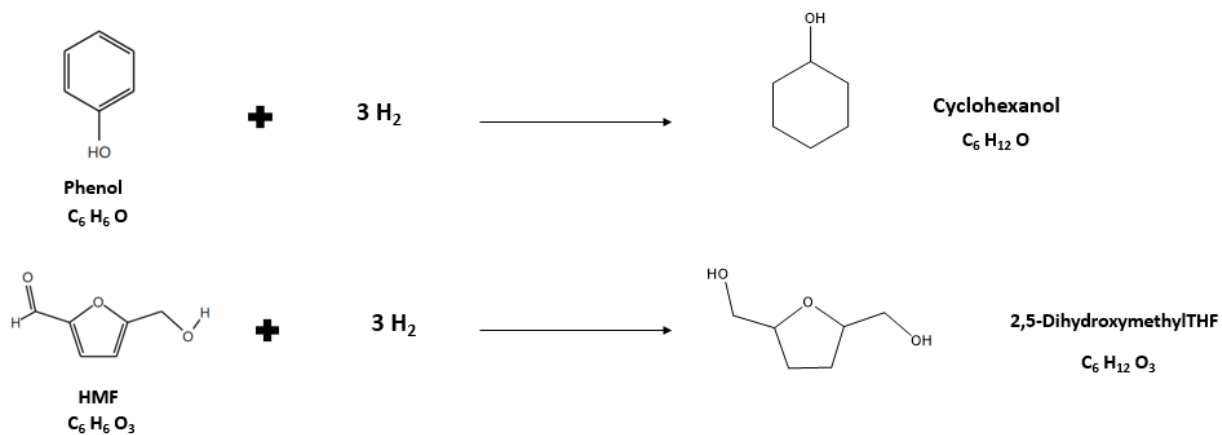


Figure 3. Representative Hydrogenation Reactions

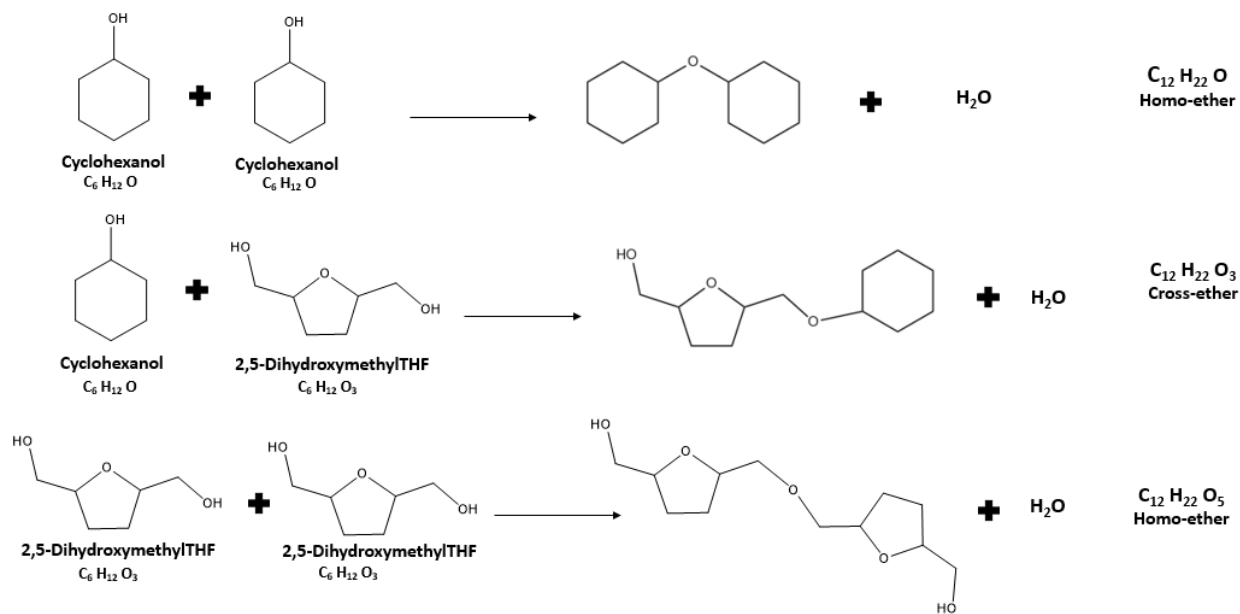


Figure 4. Representative Etherification Reactions



### 3.3 Hydrogen Production

The steam reforming and partial oxidation of NCGs were compared to meet the hydrogen demand for the hydrogenation process. The partial oxidation of NCGs was done at 1000 °C in presence of a Pt catalyst and steam reforming pathway conditions were 900°C, 20 bar in presence of Ni catalyst. Comparing the ASPEN modeling results of two hydrogen production pathways, the simulation has shown that the steam reforming approach is more efficient as it yields a high amount of hydrogen. Dry reforming of the non-condensable gases (e.g. methane) has been reported as an inefficient pathway for hydrogen production due to the water-gas shift reaction, in which a considerable portion of hydrogen reacts with carbon dioxide to produce water. Accordingly, this pathway has not been considered for the hydrogen production process [21].

In the current study, the steam reforming pathway was adopted for on-site hydrogen generation. Non-condensable gases, after being separated from pyrolysis oil, along with steam were sent to the reformer. The mass flow rate of steam to NCGs was assumed at 3:1. The products of the reformer were then cooled down to 25°C and the hydrogen was purified using a pressure swing adsorption (PSA).

### 3.4 Energy Generation

The remaining hydrogen after meeting the hydrogen demand of the hydrogenation process and char were combusted to produce heat for meeting the thermal energy demand of the process. The excess heat will be used to generate electricity. Note that only the combustion of hydrogen and char were modeled using Aspen Plus.

## CHAPTER 4: ENERGY AND MASS YIELDS

2000 dry metric tons per day of biomass was assumed in this model. The pyrolysis oil mass yield is 53.2 (wt. %) with a lower heating value of 18.151 (MJ/kg). In this process, the liquid oil from the hydrogenation reactor (intermediate product) and also the final product of the etherification reactor both have the same mass yield as bio-oil. The mass yields of oil in the whole process are equal to 53.2 as it was assumed there is no mass loss during the hydrogenation and etherification processes. About 7.5 wt. % of the produced pyrolysis char is combusted to provide sufficient energy for the pyrolysis reactor to increase the temperature of wet biomass from 25°C to 500°C. The pyrolysis oil upgrading process needs 2 wt. % of produced char to be combusted to meet the heat demand of the process. About 90 wt. % of char is used to supply the required energy for the steam reforming process of NCGs for hydrogen production. About 68 wt. % of produced pure hydrogen through the steam-reforming pathway is used to meet the hydrogen demand of the integrated pathway of fuel blendstock production. To provide the energy demand of the process after using char and excess hydrogen, 2.87 MW of electricity is imported from grid and in order to meet 429 MJ/kg heat demand of the process natural is used.

## CHAPTER 5: ECONOMIC BASELINE

The following section provides a detailed description of how the simulated model and process design are used to evaluate the renewable diesel blendstock production economics. First, total capital investment (TCI) was calculated using a comprehensive list of operating equipment in the simulated process. The annual operating costs of the process were calculated considering the variable and fixed costs. Finally, to determine the minimum fuel selling price (MFSP) a discounted cash flow analysis method was used which sets the net present value to zero at a presumed nonzero discount rate or internal rate of return (IRR). The IRR was assumed to be 10%. The MFSP is the amount at which the final product of the plant should be sold to return the specified IRR[22].

### 5.1 Capital Costs

The material and energy balance of the simulated process were used to size the process equipment of a plant processing 2,000 dry metric tons per day of forest residues with a capacity factor of 0.9. The process equipment capacity was used as a basis to assess the equipment and installed costs. Dutta's capital costs (updated to 2019 U.S. dollars) were used wherever appropriate, and new equipment costs were estimated using correlations from Turton [23]. Capital equipment for pyrolysis oil upgrading was eliminated from Dutta's ex-situ upgrading scenario, and equipment for etherification was added. The capital equipment for the hydrogen production from the non-condensable gases was adjusted to the hydrogen production rates in this process.

The total capital equipment costs, which is the sum of all equipment and installed costs, were used as a basis to calculate the total direct and indirect costs. The factors used to assess the total

direct and indirect costs and the total capital investment of the 2,000 dry metric tons per day plant are shown in Table 7.

Table 7. Capital Costs Estimates

Process Area	Assumptions	Installed Cost(MM\$/y)
Capital Equipment TIC		\$225
Warehouse	4.0% of ISBL	\$9
Site development	10.0% of ISBL	\$23
Additional Piping	4.5% of ISBL	\$10
<b>Total Direct Costs (TDC)</b>		<b>\$266</b>
Prorateable expenses	10.0% of TDC	\$27
Field expenses	10.0% of TDC	\$27
Home office & construction fee	20.0% of TDC	\$53
Project contingency	10.0% of TDC	\$27
Other costs (start-up, permits, etc.)	10.0% of TDC	\$27
<b>Total Indirect costs</b>		<b>\$160</b>
<b>Fixed Capital Investment (FCI)</b>		<b>\$426</b>
Land		\$1.8
Working Capital	5% of FCI	\$21
<b>Total Capital Investment (TCI)</b>		<b>\$450</b>

## 5.2 Operating Costs

The annual operating costs are calculated as the sum of variable and fixed operating costs. The variable costs include feedstock transportation and handling costs, catalyst cost needed for the hydrogen production process, and waste treatment (Ash disposal and water treatment) costs. Employee salaries, insurance, taxes, overhead, and maintenance costs are included in fixed operating costs. The summary of operating costs is presented in Table 8.

Table 8. Operating Costs (\$MM/y)

<b>Operating costs</b>	<b>Value</b>
<b>Variable costs</b>	<b>(\$MM/y)</b>
a. Raw materials	
Wood	\$58
H <sub>2</sub> Production catalyst	\$5
Boiler Chemicals	\$0.003
Make-up water and chemicals	\$0.141
b. Utilities	
Natural gas	\$0.371
LPS	\$0
MPS	\$0
Cooling Water	\$0.046
Electricity	\$1.6
c. Waste treatment	\$0.14
Ash disposal	\$0.475
Caustic	\$0
Others	\$0.19
d. Operating labor	\$6.2
<b>Fixed costs</b>	
e. Benefits and general overhead	\$5.6
f. Maintenance	\$13
g. Insurance and taxes	\$3
<b>Totals</b>	<b>\$93</b>
Revenue generated from electricity	\$0
<b>Net Operating costs</b>	<b>\$93</b>

### **5.3 Base case Techno-economic Analysis Results**

Techno-economic analysis indicates that 2,000 dry metric tons per day of forest residues can produce 622 metric tons per day of renewable diesel blendstock which equates to 54.1 million diesel-gallon-equivalent per year (DGE/yr.) Table 9 represents the economic assumptions for evaluating the MFSP of the final product using the discounted cash flow analysis. Modified Accelerated Cost Recovery System (MACRS) was considered for depreciation computation over a 7-year recovery period. The federal tax rate in this study was 35%. The construction period is 3 years with a 10% interest rate and all the costs analysis is for 2019 with the plant cost index of 607.4 (CEPCI = 607.4). The assessed MFSP of diesel blendstock for the base case is estimated at \$2.99 per DGE. In other words, a selling price of \$2.99 is essential to make the NPV zero.

Table 9. Economic Assumptions for MFSP Estimation for 2000 MTPD Plant

<b>Economic Assumptions</b>	<b>Value (\$MM/y)</b>
<b>Fixed Capital Investment</b>	\$426
<b>Equity</b>	40%
<b>Loan Interest</b>	8.0%
<b>Loan Term, years</b>	10
<b>Annual Loan Payment</b>	\$38
<b>General Plant</b>	\$426
<b>Steam Plant</b>	\$0
<b>Working Capital (% of FCI)</b>	10.00%
<b>Salvage Value</b>	
<b>General Plant</b>	\$0
<b>Type of Depreciation</b>	MACRS
<b>General Plant</b>	200
<b>Depreciation Period (Years)</b>	
<b>General Plant</b>	7
<b>Construction Period (Years)</b>	3
<b>% Spent in Year -3</b>	8.00%
<b>% Spent in Year -2</b>	61.00%
<b>% Spent in Year -1</b>	31.00%
<b>Start-up Time (Years)</b>	0.25
<b>Revenues (% of Normal)</b>	50%
<b>Variable Costs (% of Normal)</b>	75%
<b>Fixed Cost (% of Normal)</b>	100%
<b>Annual Interest rate</b>	10.00%
<b>Income Tax Rate</b>	35.00%
<b>Diesel Production Rate (MMgal/yr)</b>	54.1
<b>Co-product production Rate (tonne/year)</b>	0
<b>General Project life (years)</b>	30
<b>Cost Year for Analysis</b>	2019

## **CHAPTER 6: WELL-to-WHEELS LIFE CYCLE ANALYSIS**

The LCA approach is used to estimate the GHG emissions and energy consumption of the biofuel blendstock process. The well-to-wheel LCA has been conducted using Argonne's GREET 2019 software to assess environmental sustainability for producing renewable diesel fuel blendstock.

### **6.1 Base case Life Cycle Analysis Results**

Figure 5 shows the simulated renewable diesel blendstock pathway consisting of 4 processes. Production of one-gallon diesel equivalent of fuel blendstock via integrated pyrolysis, mild hydrogenation, and etherification was defined as the functional unit. 2,000 tonnes of forest residues were harvested and collected which consumed 5,280 gallons of conventional diesel. The forest residues have then transported an average of 46 miles to the biorefinery which required 758 gallons of conventional diesel. In the biorefinery section, the forest residues were pyrolyzed and etherified to produce a renewable diesel blendstock that the products include 24.6 TJ of renewable diesel blendstock and 7.2 TJ of bio-char, and 0.24 TJ electricity were imported. Finally, the renewable diesel blendstock was transported 200 miles to the pump consuming 1,460 gallons of conventional diesel. All the calculations are on a basis of 1 Diesel Gallon Equivalent (136.4 MJ/gal).



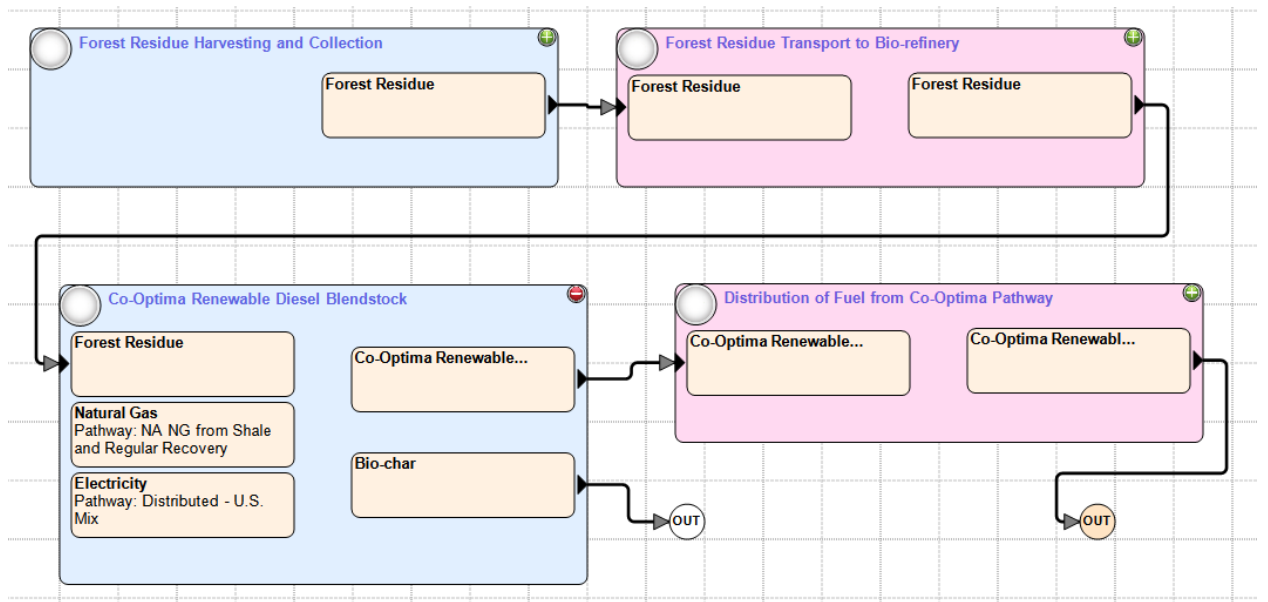


Figure 5. Renewable Diesel Blendstock Pathway Simulated in GREET 2019

Table 10 shows the comparison in energy usage and greenhouse gas emissions between the conventional diesel and renewable fuel blendstock. The results illustrate that the renewable diesel blendstock has a 93% reduction in total fossil fuel energy use and a 93% reduction in greenhouse gas emissions and a 99% of CO<sub>2</sub> reduction relative to conventional diesel.

Table 10. Comparison of Renewable Diesel Blendstock to Conventional Diesel

Energy use	Units	Conventional Diesel	Blendstock	% Reduction
Total Fossil Fuel	MJ/ DGE	164.4	11.9	<b>93%</b>
Coal	MJ/ DGE	2.1	1.2	
Natural Gas	MJ/ DGE	18.6	3.1	
Petroleum	MJ/ DGE	143.8	7.6	
<b>Emissions</b>				
Volatile Organic Compounds	g/ DGE	6.3	5.9	6%
Carbon Monoxide	g/ DGE	19.0	18.7	1%
Nitrogen Oxides	g/ DGE	131	131	0%
Particulate Matter 10 mm	g/ DGE	4.0	3.9	2%
Particulate Matter 2.5 mm	g/ DGE	3.8	3.8	1%
Sulfur Oxide	g/ DGE	3.4	2.9	15%
Methane	g/ DGE	23	23	2%
Nitrous Oxide	g/ DGE	0.3	0.3	2%
Carbon Dioxide	g/ DGE	11828	89	<b>99%</b>
Greenhouse Gases (CO <sub>2</sub> e)	g/ DGE	12639	881	<b>93%</b>

## CHAPTER 7: SENSITIVITY ANALYSIS

### 7.1 Minimum Fuel Selling Price

The MFSP sensitivity to economic assumptions for a  $\pm 1\%$  change in feedstock price, interest rate, contingency, plant size, net operating cost, fixed capital investment (FIC), and equity was determined and represented in Figure 6. In this study, the most sensitive contributor to economics and MFSP is plant size which is 2000 tonne/day. It can be predicted that by increasing the plant size, the minimum selling price decreases which means scaling up can significantly affect the MFSP. Moreover, equity is the least sensitive parameter to economics.

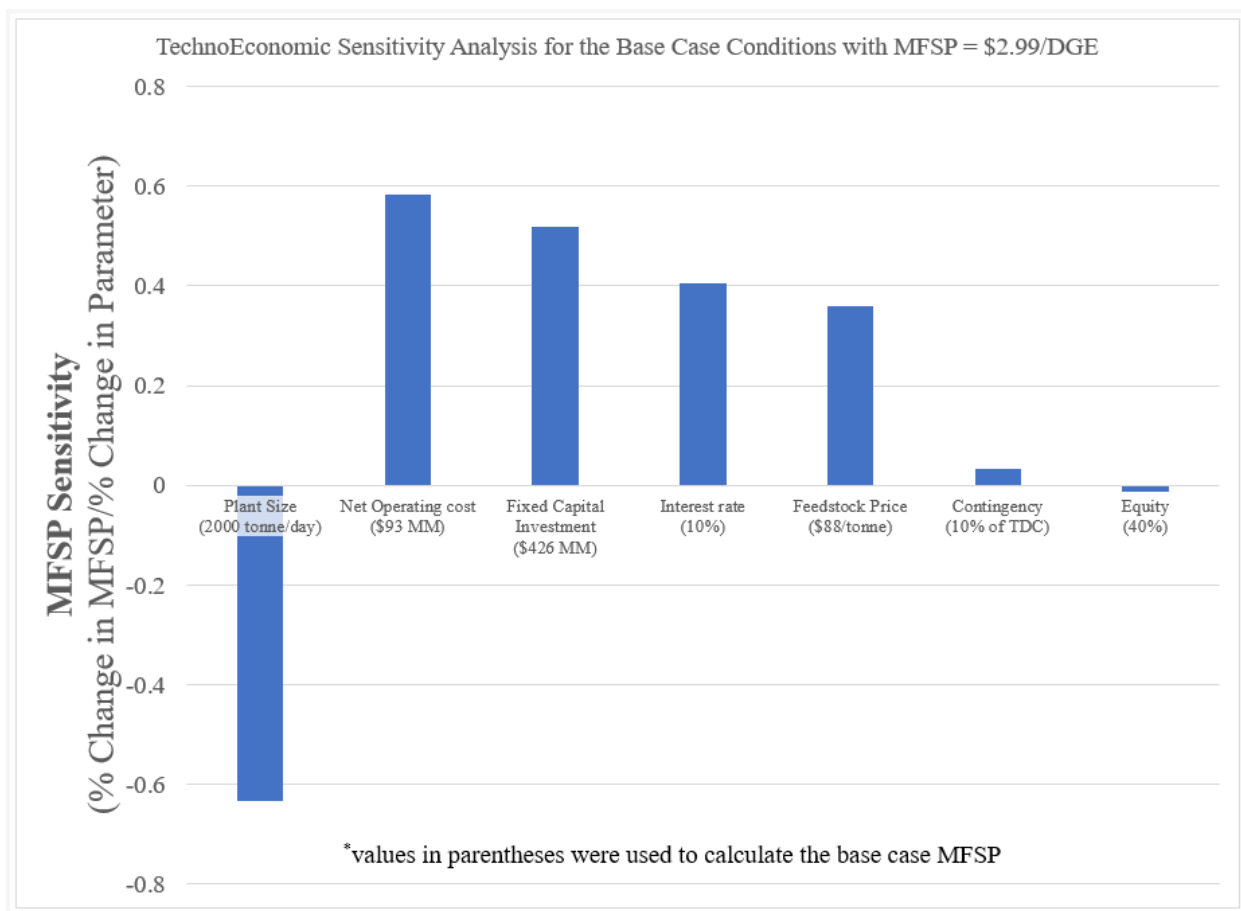


Figure 6. MFSP Sensitivity to Economic Assumptions

## 7.2 Process Condition

The effects of pyrolysis conditions on the yield, quality, and MFSP for the diesel blendstock were determined. It was assumed that the carbon, hydrogen, and oxygen composition of bio-oils do not change with pyrolysis temperature. The chemical composition of pyrolysis oils at different pyrolysis temperatures was determined from Lyu et al.'s publication [20]. The change in the chemical composition of pyrolysis oil at different temperatures is shown in Figure 7.

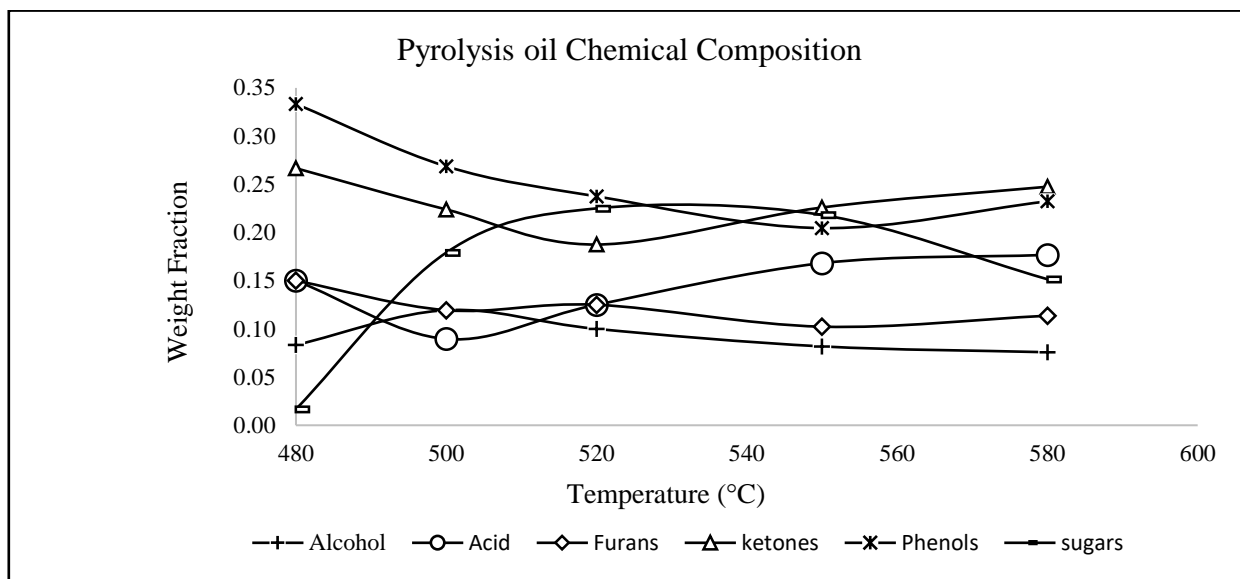


Figure 7. Reference Pyrolysis Oil Chemical Composition

Also, figure 8 presents the change in pyrolysis mass yields at different pyrolysis temperatures. The pyrolysis mass yields at different temperatures were determined by applying the residual error method in Excel. With the increase in the fast pyrolysis temperature, the bio-oil yields decreased while the char yields increased and water and NCGs yields remained constant. NCGs are formed as a result of cellulose and hemicellulose degradation during the pyrolysis process and the yields of NCGs mainly affected by the composition and moisture of the biomass. NCGs mostly contain CO and CO<sub>2</sub> and since it was assumed that the carbon, hydrogen, and oxygen composition of the bio-oils do not change with pyrolysis temperature, the yields of the NCGs and water remained constant at different pyrolysis temperatures.

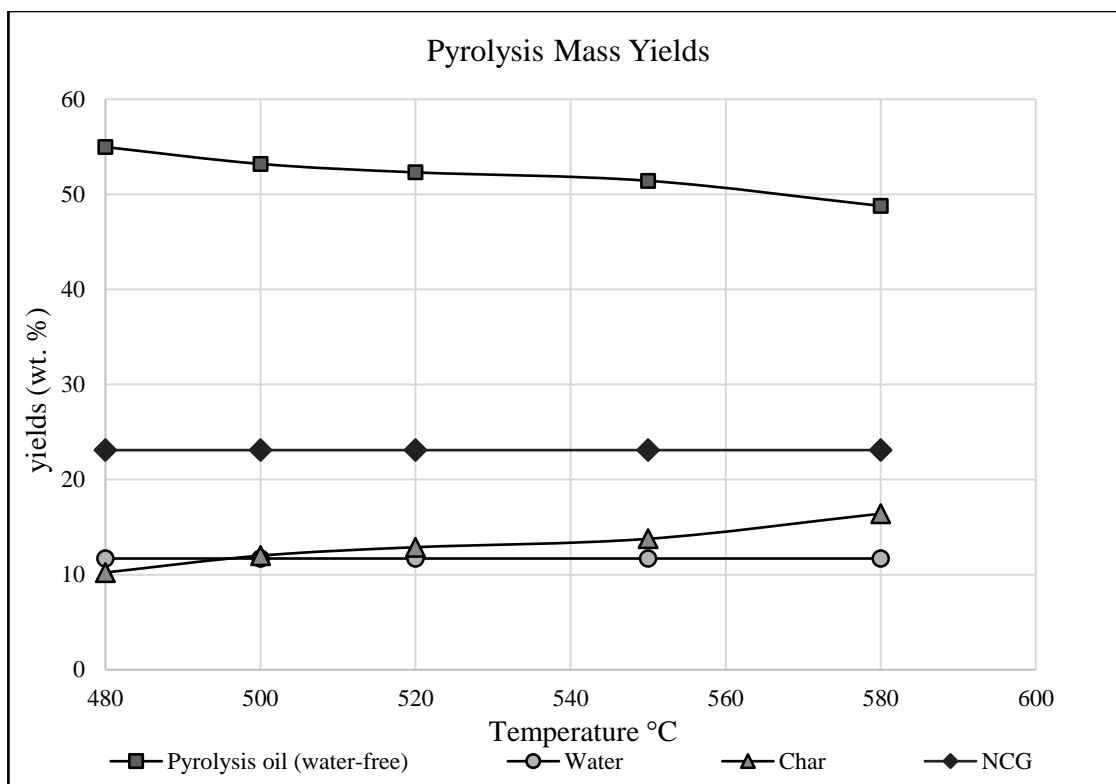


Figure 8. Pyrolysis Mass Yields vs. Pyrolysis Temperature

The lower heating values (LHV) of the diesel blendstock were assessed using Dulong's equation. The LHV of the diesel blendstock produced in the base case is 23.33 MJ/kg. The effect of temperature on the LHV of diesel blendstock is shown in Figure 9.

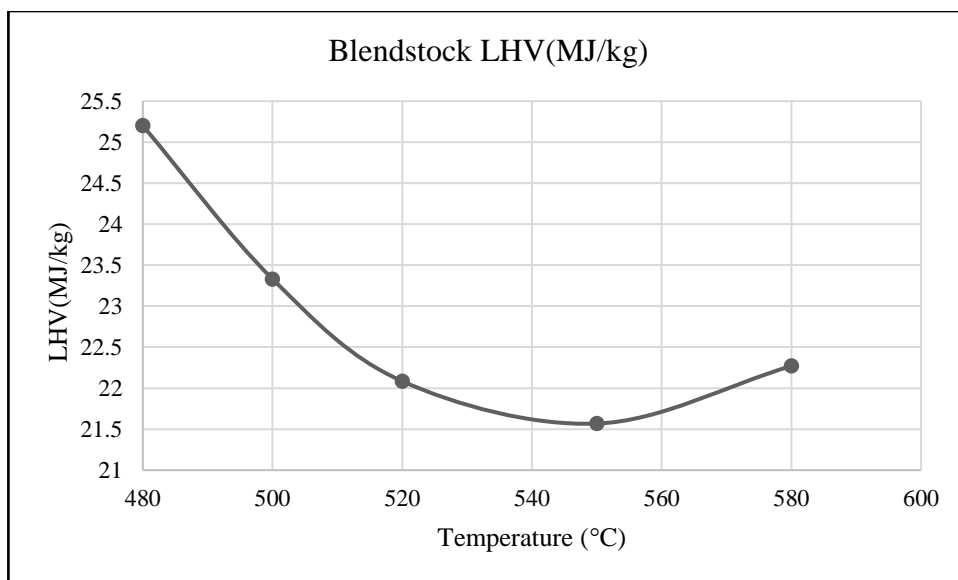


Figure 9. Blendstock Lower Heating Values vs. Pyrolysis Temperature

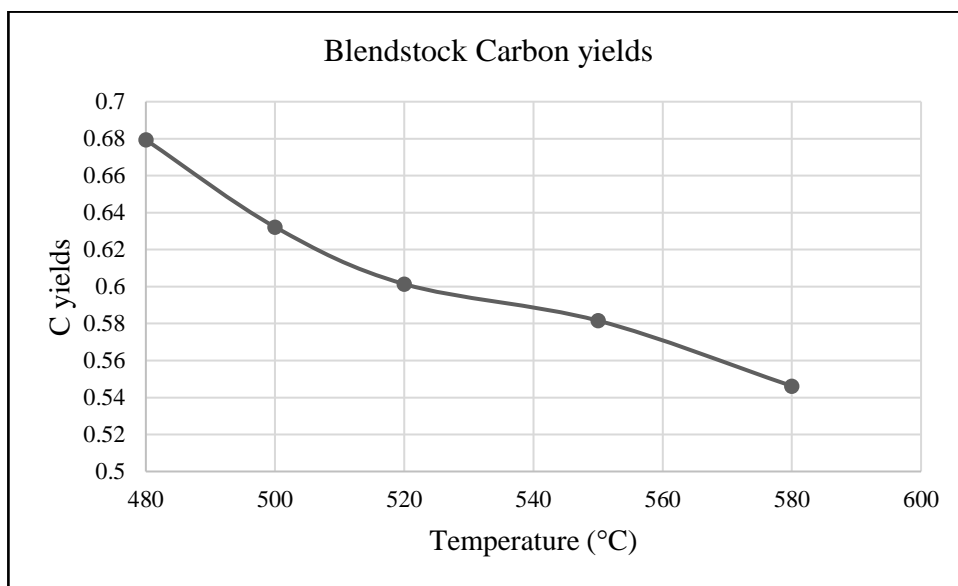


Figure 10. Diesel Blendstock Carbon Yields vs. Pyrolysis Temperature

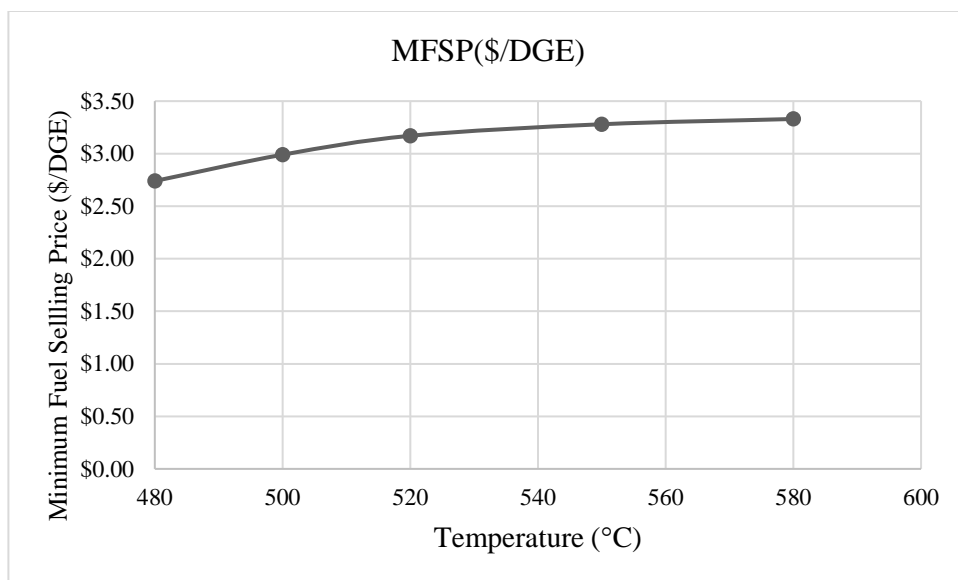


Figure 11. Minimum Selling Price (\$/DGE) of Diesel Fuel Blendstock vs. Pyrolysis Temperature

The higher value of LHV (25.2 MJ/kg) of diesel blendstock at 480 °C is due to the enriched composition of phenols and furans in bio-oil (Figure 7). The trend for carbon yields of the blendstock vs. temperature is shown in Figure 10. It is found from Figure 11 that the MFSP of diesel fuel blendstock increases with the increase in fast pyrolysis temperature, which is attributed to the decrease in LHV and carbon yields of the diesel fuel blendstock with the increase in the fast pyrolysis temperatures. In this research, fast pyrolysis temperature of 480°C to produce diesel blendstock via the etherification process results in a diesel fuel blendstock MFSP of \$2.74 which is 8 % lower than the base case (Figure 11).



## CHAPTER 8: CONCLUSIONS

The present study evaluated the economic viability and environmental sustainability of the renewable diesel blendstock production from pine sawdust through integrated fast pyrolysis and bio-oil etherification processes.

Based on the current techno-economic analysis, it was determined that diesel blendstock products can potentially be obtained from forest residues at a minimum selling price of \$2.99/DGE with a lower heating value of 23.33 MJ/kg for the baseline. Removing a low amount of oxygen through an upgrading process makes this model process economically more feasible.

Using non-condensable gases instead of natural gas to provide the hydrogen demand of the hydrotreating stage is a great advantage of this process to other processes that have been mentioned earlier. The LCA results determined that the renewable diesel blendstock has a 93% reduction in total fossil fuel energy use and a 93% reduction in greenhouse gas emissions and a 99% of CO<sub>2</sub> reduction relative to conventional diesel.

The results of the sensitivity analyses indicate that plant size (2000 tonne/day) is the most significant contributor to the MFSP of the renewable fuel blendstock. Furthermore, pyrolysis temperatures highly affect the pyrolysis oil composition and the blendstock quality. It was determined that the pyrolysis temperature of 480 °C results in the highest LHV (25.2 MJ/kg) and lowest MFSP (\$2.74/DGE) of the final product. The better product quality and a reduction in MFSP are due to the enriched composition of phenols and furans in pyrolysis oils produced at 480 °C.

## **CHAPTER 9: FUTURE WORK**

In the current study, as mentioned before, the effect of different pyrolysis temperatures on the yield, quality, and MFSP of the final product was investigated. The pyrolysis temperature is found to significantly affect the MFSP of the fuel blendstock as the pyrolysis oil chemical composition and blendstock quality change considerably with the pyrolysis temperature.

Future research is recommended to consider the potential effects of downstream process conditions particularly the effect of temperatures on the upgrading section (hydrogenation and etherification). The hydrogenation and etherification process temperatures may impact the yields and LHVs of the produced blendstock and thus influence yield, MFSP, GHG, and energy consumption of renewable fuel blendstock production.

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Appendix A: Total Equipment Installed Costs

Equip ID	Required	Spares	Equipment Name	Scaling Stream	Design Flow (per unit)	Design Flow (total)	Actual Flow (total)	Units	Size Ratio	Original Equip Cost (per unit)	Base Year	Total Orig Equip Cost (Req+Spare) in Base Year	Scaling Exp.	Scaled Cost in Base Year	Install Factor	Installed Cost in Base Year	Installed Cost in 2019\$	Scaled Uninstalled Cost in 2019\$
Feed Handling & Drying																		
C-101			Hopper Feeder	included w/ feedstock cost						INCLUDED								
C-102			Screeners Feeder Conveyor	included w/ feedstock cost						INCLUDED								
C-103			Radial Stacker Conveyor	included w/ feedstock cost						INCLUDED								
C-104			Dryer Feed Screw Conveyor	included w/ feedstock cost						INCLUDED								
C-105			Biomass Feed Screw Conveyor	included w/ feedstock cost						INCLUDED								
K-101	2		Flue Gas Blower	A100.A100DWPT.W-k110	204	408	390	HP	0.96	\$59,300	2013	\$118,600	0.78	\$114,558	1.94	\$221,775	\$237,451	\$122,655.54
M-101			Hydraulic Truck Dump with Scale	included w/ feedstock cost						INCLUDED								
M-102			Hammer mill	included w/ feedstock cost						INCLUDED								
M-103			Front End Loaders	included w/ feedstock cost						INCLUDED								
M-104	2		Cross Flow Pellet Dryer	STRM.A100.100	102,066	204,131	204,131	LB/HR	1.00	\$50,000	2011	\$100,000	0.80	\$100,000	2.00	\$200,000	\$207,410	\$103,705.16
S-101			Magnetic Head Pulley	included w/ feedstock cost						INCLUDED								
S-102			Vibratory Conveyor	included w/ feedstock cost						INCLUDED								
T-101			Dump Hopper	included w/ feedstock cost						INCLUDED								
T-102			Hammer mill surge bin	included w/ feedstock cost						INCLUDED								

Table Continued

T-103			Dryer Feed Bin	included w/ feedstock cost						INCLUDED								
T-104			Dried Biomass Hopper	included w/ feedstock cost						INCLUDED								
T-105			Lock Hopper	included w/ feedstock cost						INCLUDED								
T-106			Feed Hopper	included w/ feedstock cost						INCLUDED								
A100	1		Pinch Exchanger CAPEX								2008	\$0		\$0	2.64	\$0	\$0	\$0
												\$218,600		\$214,558	1.97	\$421,775	\$444,862	\$226,361

Fast Pyrolysis																		
C-212	2		Fines purge cooler	Included						INCLUDED								
K-211	2		Fluidizing gas recycle compressor	A200.A211.W-K211	3,648	7,296	2,886	HP	0.40	\$4,700,000	2014	\$9,400,000	0.90	\$4,079,942	1.60	\$6,527,906	\$6,882,573	\$4,301,608.17
K-212	2		Combustor air compressor	A200.A211.CHAR-COM.W-K212	10,000	20,000	13,584	HP	0.68	\$2,600,000	2014	\$5,200,000	0.78	\$3,845,515	1.60	\$6,152,824	\$6,487,112	\$4,054,445.12
R-211	2		Fluidized Bed Reactor	VOLFLMX.A200.A211.211p	1,222,474	2,444,948	2,434,448	CUFT/HR	1.00	\$3,449,500	2011	\$6,899,000	0.50	\$6,884,170	4.01	\$27,605,523	\$28,628,299	\$7,139,226.73
R-212	2		Char Combustor	VOLFLMX.A200.A211.CHAR-COM.226p	719,240	1,438,480	1,429,542	CUFT/HR	0.99	\$3,483,784	2011	\$6,967,568	0.50	\$6,945,888	3.97	\$27,569,755	\$28,591,206	\$7,203,230.94
R-212C	2		Sand Cooler	A200.A211.CHAR-COM.Q-STM212	3,671,901	7,343,802	7,359,390	BTU/HR	1.00	\$623,441	2011	\$1,246,882	0.80	\$1,248,999	3.00	\$3,746,997	\$3,885,822	\$1,295,273.91
S-211	2		Primary Cyclone	included						INCLUDED								
S-212	2		Secondary Cyclone	included						INCLUDED								
S-213	2		Char Combustor Primary Cyclone	Included						INCLUDED								
S-214	2		Char Combustor Secondary Cyclone	Included						INCLUDED								
T-211	2		Bed Media Bin	Included						INCLUDED								
T-212	2		Depleted bed media and ash storage bin	Included						INCLUDED								
T-217	2		Char combustor bed media feed bin	Included						INCLUDED								
A211	1		Pinch Exchanger CAPEX								2008	\$1,841,846		\$1,841,846	2.64	\$4,853,940	\$5,123,884	\$1,944,278
Product Condensation and Separation												\$31,555,296		\$24,846,360	3.08	\$76,456,945	\$79,598,896	\$25,938,062
D-301	1		Heavy Fraction Condenser Absorber	d301dft		12.0	12	ft	0.97	\$1,085,800	2013	\$1,085,800	0.60	\$1,068,760	1.40	\$1,494,965	\$1,600,637	\$1,144,306.13

Table Continued

D-302	1		Light Fraction Condenser Absorber	d302dft		13.0	13	ft	0.96	\$1,085,300	2013	\$1,085,300	0.60	\$1,062,244	1.33	\$1,408,332	\$1,507,880	\$1,137,328.97
H-313	1		D-301 Vapor ACHE	a300.a310.qa-h313		61,000,000	76,518,913	BTU/HR	1.25	\$578,900	2013	\$578,900	0.60	\$663,234	1.32	\$873,810	\$935,576	\$710,115.40
H-314	1		D-302 Feed Cooler	a300.a310.qc-h314		12,067,840	11,984,152	BTU/HR	0.99	\$172,000	2013	\$172,000	0.70	\$171,164	2.03	\$347,105	\$371,640	\$183,263.03
H-315	1		D-302 Feed/overhead exchanger	a300.a310.qx-h315		4,850,345	4,839,263	BTU/HR	1.00	\$758,400	2013	\$758,400	0.70	\$757,187	1.52	\$1,151,455	\$1,232,846	\$810,708.88
H-316	1		D-302 Liquid feed chiller	a300.a310.qch-h316		10,138,754	10,281,000	BTU/HR	1.01	\$132,400	2013	\$132,400	0.70	\$133,698	2.33	\$311,725	\$333,760	\$143,148.08
H-320	1		Heavy fraction ACHE	a300.a310.qa-h320		280,000	285,947	BTU/HR	1.02	\$33,300	2013	\$33,300	0.60	\$33,723	2.42	\$81,724	\$87,501	\$36,106.28
H-320A	0		Heavy fraction cooler	a300.a310.qc-h320a		845,500	11,984,152	BTU/HR	14.17	\$45,300	2013	\$0	0.70	\$0	3.23	\$0	\$0	\$0.00
H-326	1	1	D-302 Quench circulation chiller	a300.a310.qch-h326		13,087,000	13,802,399	BTU/HR	1.05	\$78,300	2013	\$156,600	0.70	\$162,544	4.63	\$753,351	\$806,602	\$174,033.91
P-318	1	1	D-301 Bottoms pump	VOLFLMX.a300.a310.318		56.0	51	gpm	0.92	\$5,800	2013	\$11,600	0.80	\$10,843	4.38	\$47,486	\$50,842	\$11,609.62
P-323	1	1	Circulation filter charge pump	a300.a310.w-p323		41	42	HP	1.03	\$25,400	2013	\$50,800	0.80	\$51,837	4.61	\$239,184	\$256,091	\$55,501.01
P-329	1	1	Aqueous filter charge pump	VOLFLMX.a300.a310.329		182.0	182	gpm	1.00	\$7,500	2013	\$15,000	0.80	\$14,996	4.20	\$62,982	\$67,434	\$16,055.64
P-331	1	1	Organic product pump	VOLFLMX.a300.a310.331		124.0	119	gpm	0.96	\$6,500	2013	\$13,000	0.80	\$12,584	4.63	\$58,274	\$62,394	\$13,473.69
P-332	1	1	Quench recycle pump	a300.a310.w-p332		0.53	1	HP	1.02	\$7,800	2013	\$15,600	0.80	\$15,907	4.88	\$77,698	\$83,190	\$17,031.00
S-319	1	1	D-301 Bottoms filter	VOLFLMX.a300.a310.320		52	48	gpm	0.92	\$14,600	2013	\$29,200	0.80	\$27,251	1.84	\$50,209	\$53,758	\$29,177.29
S-322	1		D-302 Bottoms decanter	STRM.a300.a310.323		1,013,050	1,028,335	LB/HR	1.02	\$294,700	2013	\$294,700	0.70	\$297,806	1.82	\$542,457	\$580,801	\$318,856.09
S-324	2	1	Quench circulation filter	VOLFLMX.a300.a310.324		2,340.0	2,382	gpm	1.02	\$83,100	2013	\$249,300	0.80	\$252,875	1.71	\$432,413	\$462,978	\$270,749.36
S-329	1	1	Aqueous phase filter	VOLFLMX.a300.a310.329		182.0	182	gpm	1.00	\$26,500	2013	\$53,000	0.80	\$52,985	1.77	\$93,773	\$100,401	\$56,729.93
T-328	1		The organic product surge tank	VOLFLMX.a300.a310.331		1,000	955	CUFT/HR	0.95	\$48,000	2013	\$48,000	0.70	\$46,475	3.24	\$150,656	\$161,305	\$49,759.81
T-332	1		D-301 Circulation surge tank	VOLFLMX.a300.a310.332		1,000	1,529	CUFT/HR	1.53	\$48,000	2013	\$48,000	0.70	\$64,600	3.24	\$209,411	\$224,213	\$69,165.99
A310	1		Pinch exchanger CAPEX								2008	\$1,447,138		\$1,447,138	2.64	\$3,813,738	\$4,025,833	\$1,527,618
Whole Oil Hydroprocessing																		
H-410	1		Feed-effluent exchanger	a400.a410.h-410.qx-h410		22,846,147	22,872,133	BTU/HR	1.00	\$542,500	2013	\$542,500	0.70	\$542,932	2.23	\$1,208,461	\$1,293,882	\$581,309.39
H-411	1		Feed furnace	A400.A410.QF-H411		2,210,000	14,895,323	BTU/HR	6.74	\$263,800	2013	\$263,800	0.60	\$828,837	1.31	\$1,086,789	\$1,163,609	\$887,424.44
H-413A	1		HT product ACHE	a400.a410.qa-h413		1,780,000	2,065,804	BTU/HR	1.16	\$44,800	2013	\$44,800	0.60	\$48,987	1.93	\$94,693	\$101,387	\$52,449.51
H-413C	1		HT product cooler	a400.a410.qc-h413		1,452,000	1,695,857	BTU/HR	1.17	\$63,900	2013	\$63,900	0.70	\$71,236	3.20	\$227,976	\$244,091	\$76,270.87
H-444	1		Quench hydrogen stage 2 cooler	a400.a410.qc-h444		215,000	1,695,857	BTU/HR	7.89	\$21,500	2013	\$21,500	0.70	\$91,265	7.10	\$648,193	\$694,011	\$97,716.07
H-445	1		Quench hydrogen stage 3 cooler	a400.a410.qc-h445		215,000	424,672	BTU/HR	1.98	\$21,500	2013	\$21,500	0.70	\$34,623	7.10	\$245,906	\$263,288	\$37,070.73

Table Continued

K-412	1		Hydrogen makeup compressor	a400.a410.w-k412		1,051	1,192	HP	1.13	\$1,890,000	2014	\$1,890,000	0.64	\$2,049,097	1.60	\$3,278,556	\$3,456,682	\$2,160,426.44
K-442	1		Hydrogen recycle compressor	a400.a410.k-442.w-k442		146	0	HP	0.00	\$1,200,000	2014	\$1,200,000	0.90	\$4,966	1.60	\$7,946	\$8,377	\$5,235.84
P-410	1	1	HT feed pump	VOLFLMX.a400.a410.412		135.0	119	gpm	0.88	\$43,200	2013	\$86,400	0.80	\$78,087	3.58	\$279,269	\$299,010	\$83,606.58
R-410	0		Hydrotreater, 1000 psi	STRM.a400.a410.417	55,000	0	67,293	LB/HR	0.00	\$3,396,200	2013	\$0	1.00	\$0	1.50	\$0	\$0	\$0.00
R-410	1		Hydrotreater, 1500 psi	STRM.a400.a410.417	55,000	55,000	67,293	LB/HR	1.22	\$4,775,000	2013	\$4,775,000	1.00	\$5,842,288	1.53	\$8,936,436	\$9,568,115	\$6,255,253.76
R-410	0		Hydrotreater, 2000 psi	STRM.a400.a410.417	55,000	0	67,293	LB/HR	0.00	\$6,045,800	2013	\$0	1.00	\$0	1.43	\$0	\$0	\$0.00
S-410	1		Vapor KO drum	STRM.a400.a410.410		56,193	50,068	LB/HR	0.89	\$48,500	2013	\$48,500	0.70	\$44,736	3.45	\$154,317	\$165,225	\$47,898.35
S-411	1		HP HT effluent flash: 3 phase	VOLFLMX.a400.a410.422		8,028	14,418	CUFT/HR	1.80	\$373,800	2013	\$373,800	0.70	\$563,174	2.05	\$1,156,480	\$1,238,227	\$602,982.26
S-412	1		LP HT effluent flash: 3 phase	VOLFLMX.a400.a410.428		9,494	5,430	CUFT/HR	0.57	\$45,200	2013	\$45,200	0.70	\$30,568	4.99	\$152,499	\$163,279	\$32,728.20
A410	1		Pinch exchanger CAPEX								2008	\$159,918		\$159,918	2.64	\$421,443	\$444,880	\$168,812
Oil Fractionation																		
D-450	1		Gasoline column	STRM.a400.a450.451		52,557	46,490	LB/HR	0.88	\$491,900	2013	\$491,900	0.70	\$451,423	1.69	\$762,620	\$816,526	\$483,332.45
D-451	1		Diesel column	STRM.a400.a450.455		23,368	38,548	LB/HR	1.65	\$297,900	2013	\$297,900	0.70	\$422,896	1.91	\$806,328	\$863,324	\$452,789.17
H-450C	1		D-450 Condenser (startup)	a400.a450.qcn-d450		16,444,000	7,344,412	BTU/HR	0.45	\$34,700	2013	\$34,700	0.70	\$19,738	4.58	\$90,383	\$96,772	\$21,132.76
H-450R	1		D-450 Reboiler (startup)	a400.a450.qrb-d450		6,951,000	4,736,008	BTU/HR	0.68	\$50,500	2013	\$50,500	0.70	\$38,605	2.83	\$109,165	\$116,882	\$41,334.15
H-451C	1		D-451 Condenser (startup)	a400.a450.qcn-d451		3,050,000	5,265,797	BTU/HR	1.73	\$13,200	2013	\$13,200	0.70	\$19,346	6.66	\$128,826	\$137,932	\$20,713.38
H-451R	1		D-451 Reboiler (startup)	a400.a450.qrb-d451		6,951,000	4,140,909	BTU/HR	0.60	\$50,500	2013	\$50,500	0.70	\$35,142	2.83	\$99,372	\$106,396	\$37,625.93
H-454	1		Gasoline product cooler	a400.a450.qc-h454		1,731,000	890,688	BTU/HR	0.51	\$22,400	2013	\$22,400	0.70	\$14,069	4.04	\$56,839	\$60,857	\$15,062.94
H-457A	1		Diesel product ACHE	a400.a450.qa-h457		170,000	0	BTU/HR	0.00	\$29,700	2013	\$29,700	0.60	\$0	2.34	\$0	\$0	\$0.00
H-457C	1		Diesel Product Cooler	a400.a450.qc-h457		316,000	748,243	BTU/HR	2.37	\$10,300	2013	\$10,300	0.70	\$18,832	5.63	\$106,042	\$113,537	\$20,162.68
H-459	1		D-450 Overhead vapor cooler	a400.a450.qc-h459		54,900	190,312	BTU/HR	3.47	\$7,900	2013	\$7,900	0.70	\$18,860	6.30	\$118,893	\$127,297	\$20,193.66
P-450	1	1	D-450 Reflux pump	A400.A450.D-450.QCN-D450		7,190,000	12,676,041	BTU/HR	1.76	\$9,400	2013	\$18,800	0.80	\$29,591	4.31	\$127,494	\$136,506	\$31,682.81
P-451	1	1	D-451 Reflux pump	A400.A450.D-451.QCN-D451		7,436,000	4,736,008	BTU/HR	0.64	\$7,400	2013	\$14,800	0.80	\$10,316	3.96	\$40,847	\$43,734	\$11,045.42
S-450	1	1	D-450 Overhead accumulator	A400.A450.D-450.QCN-D450		7,190,000	12,676,041	BTU/HR	1.76	\$39,100	2013	\$78,200	0.70	\$116,301	4.01	\$466,098	\$499,045	\$124,522.29
S-451	1	1	D-451 Overhead accumulator	A400.A450.D-451.QCN-D451		7,436,000	4,736,008	BTU/HR	0.64	\$28,600	2013	\$57,200	0.70	\$41,711	4.34	\$180,843	\$193,627	\$44,659.02



Table Continued

A450	1		Pinch exchanger CAPEX								2008	\$482,593		\$482,593	2.64	\$1,271,809	\$1,342,539	\$509,432
Steam System & Power Generation																		
H-601	1		Steam turbine condenser	A600.A600ST.QAH601		1.00	5.62	BTU/HR	5.62	\$1,300,000	2010	\$1,300,000	1.00	\$7,306,275	1.40	\$10,228,785	\$11,279,891	\$8,057,065.08
H-603	1		Blowdown cooler	A600.QCH603		381,671	386,077	BTU/HR	1.01	\$16,780	2007	\$16,780	0.65	\$16,906	4.32	\$73,043	\$84,443	\$19,544.16
M-601	1		BFW EDI+polishing	STRM.A600.A600BF.629		300,000	323,848	LB/HR	1.08	\$1,325,000	2010	\$1,325,000	0.60	\$1,387,228	2.00	\$2,774,457	\$3,059,559	\$1,529,779.36
M-602A	1		Steam turbine generator Stage 1	WTURB1		-40,418	-15,791	hp	0.39	\$7,700,000	2010	\$7,700,000	0.70	\$3,988,074	1.80	\$7,178,533	\$7,916,197	\$4,397,886.96
M-602B	1		Steam turbine generator Stage 2	WTURB2		-40,418	-43,564	hp	1.08	\$7,700,000	2010	\$7,700,000	0.70	\$8,114,708	1.80	\$14,606,475	\$16,107,431	\$8,948,572.69
M-603	1		Startup boiler	STRM.A200.200		204,131	204,131	LB/HR	1.00	\$275,500	2013	\$275,500	0.60	\$275,500	1.69	\$466,519	\$499,495	\$294,974.33
P-601	1	1	Makeup pump	STRM.A600.A600WTR.618		80,411	6,475	LB/HR	0.08	\$6,528	2007	\$13,056	0.30	\$6,132	4.72	\$28,930	\$33,446	\$7,088.71
P-602	1	1	Condensate pump	STRM.A600.633		247,010	323,848	LB/HR	1.31	\$9,810	2007	\$19,620	0.30	\$21,281	4.61	\$98,052	\$113,355	\$24,602.09
P-603	1	1	EDI pump	STRM.A600.633		247,010	323,848	LB/HR	1.31	\$9,810	2007	\$19,620	0.30	\$21,281	4.61	\$98,052	\$113,355	\$24,602.09
P-604	1	1	Boiler feed water pump	STRM.A600.633		494,622	323,848	LB/HR	0.65	\$304,578	2007	\$609,156	0.30	\$536,474	1.35	\$725,684	\$838,943	\$620,202.64
P-605	1	1	Condensate collection pump	STRM.A600.633		247,010	323,848	LB/HR	1.31	\$9,810	2007	\$19,620	0.30	\$21,281	4.61	\$98,052	\$113,355	\$24,602.09
S-601	1		Blowdown flash drum	STRM.A600.604		9,892	6,477	LB/HR	0.65	\$47,205	2007	\$47,205	0.65	\$35,845	3.41	\$122,408	\$141,513	\$41,439.94
T-601	1		Condensate collection tank	STRM.A600.A600BF.627		500,400	323,848	LB/HR	0.65	\$28,505	2007	\$28,505	0.65	\$21,483	6.83	\$146,734	\$169,635	\$24,835.41
T-602	1		Condensate surge tank	STRM.A600.A600BF.627		500,400	323,848	LB/HR	0.65	\$27,704	2007	\$27,704	0.65	\$20,879	6.51	\$135,957	\$157,176	\$24,137.53
T-603	1		Deaerator	STRM.A600.633		494,619	323,848	LB/HR	0.65	\$53,299	2007	\$53,299	0.65	\$40,473	5.07	\$205,102	\$237,113	\$46,789.66
T-603A	1		Deaerator packed column	STRM.A600.633		494,619	323,848	LB/HR	0.65	\$18,405	2007	\$18,405	0.65	\$13,976	5.18	\$72,367	\$83,661	\$16,157.22
T-605	1		Steam drum	STRM.A600.644		494,622	323,850	LB/HR	0.65	\$104,100	2007	\$104,100	0.65	\$79,049	2.28	\$180,044	\$208,143	\$91,386.39
T-606	1		Steam turbine condensate tank	STRM.A600.A600BF.627		500,400	323,848	LB/HR	0.65	28,505	2007	\$28,505	0.65	\$21,483	6.83	\$146,734	\$169,635	\$24,835.41
A600			Pinch exchanger CAPEX								2008	\$2,727,447		\$2,727,447	2.64	\$7,187,823	\$7,587,563	\$2,879,130

Table Continued

Cooling Water & Other Utilities																		
K-701	2	1	Plant air compressor	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$87,922	2007	\$263,766	0.30	\$244,611	1.57	\$383,656	\$443,534	\$282,787.64
M-701	1		Cooling tower system	STRM.A700.715		7,506,000	2,655,195	LB/HR	0.35	\$260,852	2010	\$260,852	0.78	\$115,977	2.47	\$286,462	\$315,899	\$127,894.42
M-702	1		Hydraulic truck dump with scale	STRM.A100.101		367,437	204,131	LB/HR	0.56	\$80,000	1998	\$80,000	0.60	\$56,225	2.47	\$138,875	\$216,566	\$87,678.59
M-703	1		Flue gas scrubber	STRM.A100.112		489,600	777,920	LB/HR	1.59	\$436,250	2010	\$436,250	0.65	\$589,449	2.47	\$1,455,939	\$1,605,551	\$650,020.48
M-704	1		Flue gas stack	STRM.A100.112		939,119	777,920	LB/HR	0.83	\$169,187	2007	\$169,187	0.65	\$149,695	1.30	\$194,476	\$224,829	\$173,057.71
M-708	1		Chilled water system	sum of H-316 and H-326		28,200,000	23,226,800	BTU/HR	0.82	\$637,500	2011	\$637,500	0.60	\$567,446	1.80	\$1,021,402	\$1,059,245	\$588,469.44
M-710	1		Product loading rack			1	1			\$25,000	2011	\$25,000	1.00	\$25,000	2.47	\$61,750	\$64,038	\$25,926.24
P-701	1	1	Cooling water pump	STRM.A700.715		7,001,377	2,655,195	LB/HR	0.38	\$239,375	2007	\$478,750	0.30	\$357,917	2.14	\$765,999	\$885,550	\$413,778.00
P-702	1	1	Firewater pump	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$23,043	2007	\$46,086	0.30	\$42,739	3.70	\$158,025	\$182,688	\$49,409.52
P-703	1	1	Diesel pump	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$3,842	2007	\$7,684	0.30	\$7,126	5.39	\$38,393	\$44,386	\$8,238.14
P-704	1	1	Ammonia pump	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$3,842	2007	\$7,684	0.30	\$7,126	5.21	\$37,095	\$42,885	\$8,238.14
P-705	1	1	Caustic pump			1	1			\$4,906	2007	\$9,812	0.30	\$9,812	4.30	\$42,200	\$48,786	\$11,343.37
P-707	1	1	BFW chemical pump	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$3,842	2007	\$7,684	0.30	\$7,126	5.21	\$37,095	\$42,885	\$8,238.14
P-708	1	1	Flue gas scrubber circulation pump	STRM.A100.112		489,600	777,920	LB/HR	1.59	\$12,510	2007	\$25,020	0.30	\$28,749	4.12	\$118,349	\$136,820	\$33,235.33
P-790	1	1	Gasoline product pump	VOLFLMX.453		108.0	53	gpm	0.49	\$7,400	2013	\$14,800	0.80	\$8,401	3.96	\$33,265	\$35,616	\$8,995.15
P-792	1	1	Diesel product pump	VOLFLMX.456		108.0	70	gpm	0.65	\$7,400	2013	\$14,800	0.80	\$10,476	3.96	\$41,478	\$44,409	\$11,216.03
S-701	1	1	Instrument air dryer	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$8,349	2002	\$16,698	0.60	\$14,361	2.47	\$35,471	\$54,462	\$22,049.40
T-701	1		Plant air receiver	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$21,005	2007	\$21,005	0.65	\$17,839	5.44	\$97,074	\$112,224	\$20,623.58
T-702	1		Firewater storage tank	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$229,900	2007	\$229,900	0.65	\$195,252	1.46	\$285,447	\$329,997	\$225,725.33
T-703	1		Purchased diesel storage tank	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$104,674	2007	\$104,674	0.65	\$88,899	1.35	\$119,665	\$138,341	\$102,773.26
T-704	1		Ammonia storage tank	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$15,704	2007	\$15,704	0.65	\$13,337	5.39	\$71,850	\$83,064	\$15,418.84
T-705	1		Caustic storage tank	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$16,005	2007	\$16,005	0.65	\$13,593	3.01	\$40,936	\$47,325	\$15,714.38
T-708	1		BFW chemical storage tank	STRM.A100.101		262,454	204,131	LB/HR	0.78	\$22,004	2007	\$22,004	0.65	\$18,688	6.70	\$125,186	\$144,723	\$21,604.44
T-790	1	1	Gasoline product storage tanks	VOLFLMX.453		50	53	gpm	1.06	\$442,700	2013	\$885,400	0.70	\$885,400	1.75	\$1,553,400	\$1,663,203	\$947,985.12

Table Continued

T-792	1	1	Diesel product storage tank	VOLFLMX.456		50	70	gpm	1.40	\$442,700	2013	\$885,400	0.70	\$885,400	1.75	\$1,553,400	\$1,663,203	\$947,985.12
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Water Management																		
P-860	1	1	RO Feed pump	VOLFLMX.A800.A860.860		185	170	gpm	0.92	\$6,400	2013	\$12,800	0.80	\$11,961	3.84	\$45,976	\$49,226	\$12,806.69
P-866	1	1	Clean water pump	VOLFLMX.A800.866		140	127	gpm	0.91	\$5,200	2013	\$10,400	0.80	\$9,650	4.35	\$41,940	\$44,905	\$10,332.01
T-801	1		Clarifier overflow tank			1	1		1.00	\$85,800	2013	\$85,800	0.65	\$85,800	2.27	\$195,000	\$208,784	\$91,864.83
T-809	1		Slurry tank			1	1		1.00	\$85,800	2013	\$85,800	0.65	\$85,800	2.27	\$195,000	\$208,784	\$91,864.83
T-810	1		Boiler Feed Tank	VOLFLMX.A800.A810.810		200	182	gpm	0.91	\$24,600	2013	\$24,600	0.70	\$23,022	4.49	\$103,412	\$110,722	\$24,649.36
T-812	1		Steam drum	VOLFLMX.a800.a810.813		100,800	100,772	CUFT/HR	1.00	\$24,400	2013	\$24,400	0.70	\$24,395	4.46	\$108,879	\$116,575	\$26,119.62
T-814	1		Boiler feed tank	VOLFLMX.A800.A810.822A		145	131	gpm	0.90	\$24,400	2013	\$24,400	0.70	\$22,746	4.46	\$101,519	\$108,695	\$24,354.14
T-822	1		Steam drum	VOLFLMX.a800.a810.823		156,000	155,386	CUFT/HR	1.00	\$19,400	2013	\$19,400	0.70	\$19,347	5.23	\$101,120	\$108,268	\$20,714.04
T-860	1		RO Feed tank	VOLFLMX.A800.A860.860		185	170	gpm	0.92	\$76,000	2013	\$76,000	0.70	\$71,624	2.24	\$160,211	\$171,536	\$76,686.66
T-866	1		Clean water tank	VOLFLMX.A800.866		140	127	gpm	0.91	\$194,200	2013	\$194,200	0.70	\$181,887	2.23	\$406,484	\$435,216	\$194,744.20

Etherification																		
	1		Etherification Reactor 10 m^3, WHSV 4/hr	2000 TPD capacity: Design Flow =100		100	100		1.00	\$84,000	2018	\$84,000	0.60	\$84,000	2.50	\$210,000	\$211,532	\$84,612.94
	1		Catalyst Zirconia Alibaba \$5/kg, 5500 L, rho=2.5	2000 TPD capacity: Design Flow =100		100	100		1.00	\$70,000	2019	\$70,000	0.60	0	2.50	0	0	0
	1		Heater	2000 TPD capacity: Design Flow =100		100	100		1.00	\$128,000	2018	\$128,000	0.60	\$128,000	2.50	\$320,000	\$322,335	\$128,934.00
	3		Cooler	2000 TPD capacity: Design Flow =100		100	100		1.00	\$492,000	2018	\$1,476,000	0.60	\$1,476,000	2.50	\$3,690,000	\$3,716,925	\$1,486,770.15
	1		Centrifuge	2000 TPD capacity: Design Flow =100		100	100		1.00	\$118,864	2018	\$118,864	0.60	\$118,864	2.50	\$297,160	\$299,328	\$119,731.33
Hydrogenation																		
	1		Hydrogenation reactor , WHSV 1/1.6hr	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50	\$6,800,000.00		
Steam reforming																		
	1		Steam reforming reactor	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			
	1		Heater	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			

Table Continued

	1		Pump	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			
	1		Compressor	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			
Total																\$20,000,000.00		
	1		Cooler	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			
	1		Pressure Swing Adsorption	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50			
Boiler			Boiler	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50	\$19,236,705.01		
Turbine			Generator	2000 TPD capacity: Design Flow =100		100	100		1.00				0.60		2.50	\$0.00		
Plant Total												\$77,298,896		\$73,869,251	2.28	\$167,923,330	\$224,645,559	\$84,630,156

All prices adjusted to CEPCI 2019:

**Table A.1 CEPCI values used for equipment costing**

<b>Year</b>	<b>CEPCI value</b>
<b>2006</b>	499.6
<b>2007</b>	525.4
<b>2008</b>	575.4
<b>2009</b>	521.9
<b>2010</b>	550.8
<b>2011</b>	585.7
<b>2012</b>	584.8
<b>2013</b>	567.3
<b>2014</b>	576.1
<b>2015</b>	557
<b>2016</b>	542
<b>2017</b>	568
<b>2018</b>	603
<b>2019</b>	607.4

## Aspen Plus® Process Flow Diagram



## **BIOGRAPHY**

Aysan Najd Mazhar was born in Tehran, Iran on August 16, 1989. She was raised in Karaj, Iran and graduated from Dr. Keshiafshar high school in 2007. She attended Tehran University in 2010 and graduated in 2014 with a B.S. degree in Natural Resources Engineering-Wood and Paper Science and Technology- Pulp and Paper. She pursued her studies in Tehran University and graduated with a Master's degree in Natural Resources Engineering-Wood and Paper Science and Technology- Pulp and Paper in 2016.

Aysan is a candidate for the Master of Science degree in Chemical Engineering from the University of Maine in December, 2021.