

University of Nevada, Reno

Valorization of the Organic Fraction of MSW via Hydrothermal Carbonization and Fischer-Tropsch Synthesis

A thesis submitted in partial fulfillment
of the requirements for the degree of

Bachelor of Science in Chemical Engineering and the Honors Program

by

Riley Kessinger, Kathleen Wright, Marc Nabhan, and Carlos Santiago

Dr. Charles Coronella, Thesis Advisor

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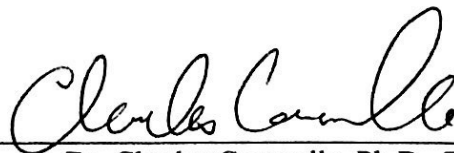
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BACHELOR OF SCIENCE, CHEMICAL ENGINEERING



Dr. Charles Coronella, Ph.D., Thesis Advisor

Erin Edgington, Assistant Director, Honors Program

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Abstract

The ability to impact the world in a positive way through the design of a process is one of the many benefits of an engineering expertise. Through chemical engineering, the world's greatest problems can be solved with enough detail and big picture views combined to make a better future. Greenhouse gases in the atmosphere produced by man contributes to climate change and the detrimental effects on the environment, which directly impacts society itself. One of the largest causes of greenhouse gas production is organic waste in landfills. The organic waste buried under trash with no oxygen in landfills undergoes anaerobic digestion and breaks down into methane gas. To combat excess greenhouse gas production and help reduce mankind's impact on the environment, a process was designed to convert organic food waste into diesel fuel using three main unit operations: hydrothermal carbonization, gasification, and Fischer Tropsch reaction. With an input feed of 1 metric ton of food waste per hour, about 250 kg of diesel precursors are produced per hour assuming perfect conversion efficiency in the reactors. A full process was designed and simulated on ChemCAD, a full economic analysis was conducted for worst case and best-case scenarios, industry standards were evaluated that applied to the process, detailed hazards were determined for the process operations, and an environmental assessment was performed for all materials used. Through the research and design of this process, companies can start to abide by new environmental laws that prohibit any organic waste from entering landfills. This process was designed entirely with chemical engineering operations and practices from start to finish, showing the broad range of skills that chemical engineers have as well as their advanced problem solving skills.

Acknowledgements

The team would like to thank Dr. Coronella for his input and expertise, which helped design this process tremendously. Without Dr. Coronella's previous knowledge and research in hydrothermal carbonization and waste-to-fuel processes, this project would have not been as successful as it turned out to be. The team would also like to thank Fulcrum Bioenergy, a company based in Pleasanton, California and operating in Sparks, Nevada, for their collaboration and helpful suggestions as the team was first defining the scope of the process. Their comments and preliminary feedback were essential and were applied at various steps of achieving this project. A final appreciation goes to the department of materials and chemical engineering at the University of Nevada, Reno for always being helpful and for offering all of the resources necessary for the realization of this work.

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I. Problem Description

Humans all around the globe produce an enormous amount of solid waste. In 2016, the world generated 1.3 billion tonnes of municipal solid waste, with just the United States generating 262.4 million tonnes¹. Organic waste buried in landfills undergoes anaerobic digestion, breaking down the organic molecules into greenhouse gases such as methane. As landfills begin to run out of space for waste storage and greenhouse gases pollute the atmosphere, alternative uses for waste material need to be put in place in order to prevent ecological disaster. In general, conversion of waste to energy is not pursued due to the large capital cost of the process and the low quality of the fuel that is produced. New laws such as AB 1826 (mandatory commercial organics recycling in California) are being implemented to combat the solid waste problem in the United States¹. As these types of laws become the new standard around the country and around the globe, conversion of waste to energy may become more sought out and might consist of a more economically viable business model. Companies need to find a sustainable option for their food waste rather than sending it to a landfill in order to comply with the recycling laws that limit landfill dumping and biofuels could be the best option, especially that new technology and new findings are making the process increasingly attractive.

To provide way that diverts organic waste from landfills, the team designed a process for converting organic solid municipal waste into hydrocarbon fuel using three main unit operations of hydrothermal carbonization, gasification, and Fischer-Tropsch reactions. Pure food waste that is normally composted could instead be fed to the process to produce biodiesel. Biodiesel is an alternative fuel source that significantly reduces

greenhouse gases, sulfur dioxide in air emissions, and asthma-causing soot. The team was responsible for designing this process as a green field, simulating it with process design software, and determining various process constraints to comply with environmental laws, make the most money, and identify all possible hazards. The deliverables for the project include a working ChemCAD model, a greenfield economic analysis, an industry standard analysis, a HAZOP, and recommended operating conditions.

II. Project Constraints

The primary constraints that apply to designing this process are the type of waste entering the process, the amount of waste being used up, the appropriate unit operations and their own constraints, and the type of fuel being produced. Organic waste is a broad category that includes many different biodegradable materials such as food scraps, plant waste, sewage, slaughterhouse waste, cardboard, and biodegradable plastics. Any of these materials could potentially enter the process to be converted into fuel; however, the more diverse the feed, the more difficult the process. The team determined that a significant amount of extra labor, multiple separation operations, autoclaves, and an unknown chemical composition would be needed in order to pull waste from a landfill rather than a more purified food waste feed acquired from grocery stores, restaurants, universities, and hospitals. So, food waste as the feed would be the most economically viable decision.

This constraint helped the design of the process because an estimated composition analysis could be done for the amount of elements in the food input, which was necessary to accomplish an overall mass balance for the process and input a specific feedstock composition into ChemCAD. The basis for feedstock entering the process was a

constraint because the sizing of the unit operations are directly dependent on how much material is being processed. A few different basis were applied to compare economics in the model. Initially 1000 kg/hour of food waste was chosen, with this number scalable if needed to be increased. The sizing of the unit operations were done with this basis, and if the feed were to be increased, the operations could be equivalently increased. This basis would produce 250kg of the desired product (waxy hydrocarbons) per hour . The constraint of what type of product to produce was determined by what would yield the most revenue and what could be obtained from the FT reactor. In order to make diesel product, heavier hydrocarbons known as waxes are required to be produced that can be refined into diesel fuel. This was chosen as the product because diesel can be produced easily in a low temperature FT reactor.

In order to produce the chosen diesel product, constraints were applied to each of the main unit operations. The process needed to include a hydrothermal carbonization reactor, a gasifier, and a Fischer Tropsch reactor. The Fischer-Tropsch reactor can run with different specifications depending on the desired input and output. An iron catalyst was chosen as a constraint for this reactor because it can internally produce a water gas shift reaction to created the desired hydrogen to carbon monoxide ratio. Iron is also cheapest compared to cobalt and rubidium and can work under both high temperature reactions and low temperature reactions. This was the next constraint to be chosen. Low temperature FT synthesis was chosen because lower temperatures produce longer hydrocarbon chains, the desired product of waxy hydrocarbons. Next, there are many types of gasifiers that could be used in this process. An entrained flow GE gasifier was

chosen with reference to a published paper because the team knew it would work for this particular process. Finally, the hydrothermal carbonization reactor could be continuous or batch, and batch was chosen due to the ease of feed input into the unit. A continuous reactor would have the added difficulty of the need for a pump capable of pushing solid waste into a high pressure reactor.

The basis of the design is the assumption of a feedstock of 1 metric ton per hour of food waste collected from various public institutions such as hospitals and schools. This feed going into the process, according to the ChemCAD simulation and the NREL report, produces about 250 kg of diesel precursors to be refined into diesel fuel.

III. Market analysis

Traditional oil and gas supply chain has three main sections: upstream (exploration and production), midstream (transportation through pipelines) , and downstream (refineries². The product from this process is nontraditional and could be considered to have a part in all of the three supply chain sections. This product made by the FT reactor consists of light hydrocarbons and waxes, but is not ready for use as diesel fuel. This commodity thus contains significant amounts of high-molecular-weight wax. Hydrogen is required to crack these high-molecular-weight paraffins to low-molecular weight hydrocarbons (typically with C12-C21 chains³. The plan is to sell that fuel precursor to a refinery that would later hydrocrack it and transform it into diesel fuel.

The market in which this product will compete is the biofuel industry. Exxon Mobil is one of the biggest corporate giants that has started considering biofuels. Their “Farm Waste to Fuel Tank” initiative makes them a big competitor in the market⁴. The fact that

they would operate the whole process from waste all the way to fuel, their production could put a halt to the sales of smaller companies and startups such as the one considered here. Nonetheless, according to Zion market research, the biofuels market size is expected to reach USD 218.7 Billion by 2022⁵. The major two fuels in that sector are bioethanol and biodiesel. Some of the top players that are taking over this said market, to name a few, are Copersucar S.A DSM, Green Plains Inc., Aemetis Inc, Western Dubuque Biodiesel Llc, Solazyme Inc, Renewable Energy Group, Raizen Energia Participacoes S.A, BlueFire Renewables, Aventine Renewable Energy Holdings, Inc. (AVRW), and Australian Renewable Fuels Ltd. among others⁵. Growth is in the horizon for this market and being a part of it as soon as possible is highly recommended. Cooperating with one of the aforementioned companies could also be wise since selling them an intermediary product could help their production line and assist them in producing slightly varying blends of fuels. For example, Australian Renewable Fuels Limited is invested in producing biodiesel in two of its plants in Australia. Their goal is to produce fuel that meets the strictest biodiesel standards. Combining their expertise on the standards and refining of biodiesel with the high volume production in Nevada caused by the strict California laws could be a winning situation. Distance could be a potential constraint here, but the in this global market, that is seldom an issue. Overall, there is a variety of routes that our project can take economically, but in general, the market prospects are positive and the global reach of the supply chain makes this project very appealing.

IV. Engineering Standards

The EPA has specific standards for what diesel can be made of, with important regulations on certain pollutants like sulfur levels. Because this process has virtually no sulfur content in the diesel, the majority of the regulations are easily satisfied, saving the producing company a lot of time and money. One of the main characterizations of diesel fuel is the cetane number, which is a measurement of the delay of ignition. A higher cetane number ignites more quickly. Diesel fuels are 75% saturated hydrocarbons and 25% aromatic hydrocarbons, with the average molecular formula being $C_{10}H_{20}$ to $C_{15}H_{28}$. The hydrocarbons made from the team's design, as simulated in ChemCAD, satisfy the standard of the average molecular formula to convert waxes into the diesel fuel for saturated hydrocarbons, shown in **Figure 2**. Ignoring water, the hydrocarbons produced are a mixture of mostly waxes with about 16 carbons, and a small percentage of various other hydrocarbons like nonane, decane, and hexane. The ChemCAD simulation had to produce the desired products in order to comply with the diesel hydrocarbon standards, so the team had to manipulate the specifications of the unit operations to achieve this goal. Hydrocarbons with more carbon chains than 16 will be sold with the waxes to produce diesel. **Figure 1** below addresses multiple different chemical properties and what they should be for diesel. These properties include not only carbon number in the molecular formula but also its heat of vaporization, nitrogen content, electrical conductivity, vapor density, flammability limits, and energy content. Although not all of these properties can

be measured in the simulation, their estimates can be inferred to meet protocol due to the nature of the reactions.

Property	Example	Property	Example
Carbon number	C12 – C20	Nitrogen, mg/kg	~30
Molecular weight range, g/mol	~150 – 250	Total aromatics, wt-%	~20
Carbon/Hydrogen, wt-%	~86.5/13.5	Stoichiometric air to fuel ratio	14.7
Distillation, °C	200 – 360	Vapor density	
LHV energy content, MJ/kg	43	Autoignition temperature, °C	230
LHV energy content, MJ/l	35	Flammability limits, vol-%	0.6 – 5.6/6.5
HHV energy content, MJ/kg	46	Electrical conductivity, $\mu\text{S}/\text{m}^*$	10^{-4}
Heat of vaporization, kJ/kg	225 – 280		

Figure 1: Diesel hydrocarbon properties ⁶

Stream No.	21	Bimethyl	7.263143e-006
Stream Name	FT Products	Propyl hydride	0.03571325
Temp C	42	Isobutane	0.1118312
Pres bar	23.58	2-Methylbutane	0.002767307
Vapor Fraction	0	Hexane	0.007010587
Enthalpy MJ/h	-3111.506	Dipropylmethane	0.009469707
Total flow	10636.88	N-Octane	0.9476078
Total flow unit	mol/h	N-Nonane	1.089899
Comp unit	weight %	N-Decane	1.213713
Water	56.84876	Hendecane	1.321575
food waste	0	Bihexyl	1.414794
hydrochar	0	Tridecane	1.493287
Carbon Dioxide	0.2558666	Tetradecane	1.557481
Carbon Monoxide	0.006303242	N-Pentadecane	1.608137
Hydrogen	0.0009562088	Cetane	1.645424
Ammonia	0	N-Octadecane	1.685322
Hydrogen Sulfide	0	N-Nonadecane	1.689352
Nitrogen	0	n-Icosane	1.684112
MDEA	0	N-C16-CycloC5	23.69968
Methane	2.59335e-006	Heptadecane	1.670934

Figure 2: FT reactor ChemCAD Hydrocarbon Results

To ensure that every country has similar standards for fuel, the automobile and engine manufacturers defined recommendations for fuels called the World Wide Fuel Charter (WWFC). Requirements for the Europe, US, and the WWFC are shown below. In the United States, ASTM D 975 is the specification for diesel fuel, which includes multiple standards shown below as Standard A and Standard B. Looking further into ASTM D 975, 7 grades of diesel fuels are specified to suit various types of diesel engines. The grades are designated mostly by ppm of sulfur. Assuming the team's process creates

diesel with virtually no sulfur content, this would be classified as either Grade No. 1-D S15, “a special-purpose, light middle distillate fuel for use in diesel engine applications requiring a fuel with 15 ppm sulfur (maximum) and higher volatility than that provided by Grade No. 2-D S15 fuel” or Grade No. 2-D S15, “A general purpose, middle distillate fuel for use in diesel engine applications requiring a fuel with 15 ppm sulfur (maximum). It is especially suitable for use in applications with conditions of varying speed and load”. To determine which grade the fuel would classify as, it must be determined whether the final product has characteristics of light middle distillate or middle distillate at a certain volatility. The team decided to restrict the process simulation to end at the FT reactor instead of further refining the product because many companies have the infrastructure in place to refine the waxy hydrocarbons through hydrocracking. This decision gave the team the ability to specify any type of diesel product rather than restricting it to one. Because the waxy hydrocarbon product will be sent to an outside company to convert into diesel, either of these classifications can be met depending on the way it is refined. There are 13 tests included in ASTM D 975 that must be met at the time of fuel delivery, also after the refining process. There are 1D or 2D specifications determined by the diesel’s density and viscosity, and either can be met using the hydrocarbon waxes. **Figure 3** summarizes which properties are specified in ASTM, and **Figure 4** specifies the properties for multiple standards.

Summary of ASTM Specifications	
Property	Importance
Cetane Number	Measure of ignitability (ignition quality), reduce knock and smoke
Cetane Index/Aromatics Limit	Limits aromatic content of fuel to prevent adverse emissions impact, reduce knock and smoke
Volatility	Deposits, wear, exhaust smoke
Viscosity	Injector wear & spray pattern, pump wear, filter damage
Sulfur Content	To protect emissions control equipment
Low Temperature Operability	Flow properties, filter plugging
Water & Sediment Content	Filter plugging, injector wear, increased corrosion
Lubricity	Injector & pump wear
Ash Content	Injector & fuel pump wear, piston & ring wear, engine deposits
Corrosion	Protect copper, brass, bronze fuel system parts
Flash Point	Safety during fuel handling & storage
Carbon Residue	Fuel system deposits, combustion chamber deposits

Figure 3: ASTM Specifications⁷

	European 2009/30/EC ^a	Standard A 2013/2017 ^a	Standard B 2014 ^a	WWFC:2013 Category 4 ^a
Cetane number	≥51.0	≥51.0 ^b	≥40	≥55.0
Cetane index		≥46.0	≥40 or aromatics ≤35 vol-%	depends on additive use
Density at 15 °C, kg/m ³	≤845.0	820 ^b – 845		820 ^b – 840
Viscosity at 40 °C, mm ² /s		2.000 ^b – 4.500	1.9 – 4.1	2.0 ^b – 4.0
CFFP, °C		^b	agreed by buyer and seller	equal or lower than the lowest expected temperature
Flash point, °C		>55.0	≥52	≥55
Evaporated, vol-%		E250: <65 E350: ≥85		
Evaporated, °C	T95: ≤360.0	T95: ≤360	T90: 282 – 338	T90: ≤320 T95: ≤340
Final boiling point, °C				≤350
Dist. residue/loss, vol-%			≤2	
Total aromatics, wt-%			Total ≤35 or CI ≥40	≤15
Polycyclic aromatic hydrocarbons (PAH di+), wt-%	≤8.0	≤8.0		≤2.0
Sulfur content, mg/kg	≤10.0	≤10.0	≤15	≤10
FAME content, vol-%	≤7.0	≤7.0	≤5.0 ^e	≤5.0
Other biofuels				HVO, BTL
Methanol/ethanol, wt-%				non-detectable
Water content, mg/kg		≤200		≤200
Lubricity, wear scar diameter (wsd 1.4) at 60 °C, μm		≤460.0	≤520.0	≤400
Copper strip corrosion (3h, 50 °C)		Class 1	≤3	Class 1
Ferrous corrosion				max. light rust
Total acid number, mg KOH/g				≤0.08
Carbon residue (10% dist.), wt-%		≤0.3	≤0.35	≤0.20
Ash content, wt-%		≤0.010	≤0.01	≤0.001
Metal content, mg/kg	≤2.0 ^d manganese	≤2.0 ^d manganese		1 or non- detectable
Oxidation stability 95 °C, g/m ³		≤25		≤25
Oxidation stability, hours		>20 ^c		
Total contamination, mg/kg		≤24		<10
Water and sediment, vol-%			≤0.05	water ≤200 mg/kg
Conductivity, pS/m			≥25	

Figure 4: Diesel Standards ⁶

Because the hydrocarbon product of the FT reactor will not be refined as part of the process but rather be sent to an outside refinery, many of the other standards in categories like diesel fuel additives, handling procedures, and engine emission standards do not need to be addressed from this process alone. The expensive testing required for quality values similar to the ones in figure 4 also does not have to be at the team's process expense because most of that is done at the time of fuel delivery.

V. Nevada Regulations & Fees

There are other regulations in place for building the waste to fuel plant to produce the diesel product. According to the Nevada Division of Environmental Protection, there are many standards for land, air, and water emissions in the state of Nevada ⁸. The Bureau of Air Quality Planning (BAQP) develops the regulations, standards, and State implementation plans to maintain the provisions of the Clear Air Act. A permit is required if the process has any type of emission source, and if more than 5 acres of land are being disturbed. A surface area distribution (SAD) permit is needed if the 5 acres of land are unrelated to agriculture. There are two classes of air total HAP and less than 10 tons per year of any one HAP. These permits also costs a certain amount per year. Assuming the team's process converts a large amount of biomass into fuel per year, the waste to fuel plant would need a class I permit. The fees for this permit and the SAD permit are shown below.

Class I Permit Fees						
("Major Sources" including Title V and PSD)						
Permit	New	Renewal	Maintenance / Annual Fee Schedule	Significant Revision	Minor Revision	Administrative Amendment
Major Stationary Source with PSD Permit	\$50,000	\$5,000	\$30,000 + \$16.98/ton	\$50,000	\$5,000	\$200
Major Stationary Source without PSD Permit	N/A	\$5,000	\$25,000 + \$16.98/ton	\$50,000	\$5,000	\$200
Class I Operating Permit	\$30,000	\$5,000	\$20,000 + \$16.98/ton	\$20,000	\$5,000	\$200
Class I Operating Permit: Landfill	\$30,000	\$5,000	\$15,000 + \$16.98/ton	\$20,000	\$5,000	\$200
Class I Operating Permit to Construct	\$20,000	No renewal. Convert to Class I Operating Permit. \$5,000 per phase.	-	\$5,000	\$5,000	\$200
Mercury Operating Permit to Construct	\$5,000	No renewal. Good for life of AQOP	Per-thermal unit fee determined annually: Fee = \$500,000 / total # thermal units permitted industry-wide.	\$5,000	\$5,000	\$200

Figure 5: Permit fees for new process⁸

Surface Area Disturbances Permit Fees						
Permit	New	Renewal	Maintenance / Annual Fee Schedule	Significant Revision	Minor Revision	Administrative Amendment
SAD	\$500	\$500	≥ 500 acres \$5,000 ≥ 200 acres but < 500 acres \$2,000 ≥ 100 acres but < 200 acres \$1,000 ≥ 50 acres but < 100 acres \$750 ≥ 20 acres but < 50 acres \$500 ≥ 5 acres but < 20 acres \$250	\$200	-	\$200

Figure 6: SAD permit costs⁸

The permits last 5 years, and to construct a class I process the construction permit lasts 12 months. The Bureau of Water Pollution Control (BWPC) has its own permitting programs and requirements to prevent pollution from entering the water in Nevada. The Clean Water Act defines most of the types of pollutants and what is classified as water of

the United States. In addition to the Clean Water Act, the state of Nevada has more comprehensive requirements. In chapter 445A of the Nevada Revised Statutes, the term waters of the state are much more detailed in what is defined as water in which polluting is illegal. The application and fees of getting a water permit are at the NDEP website⁸. The requirements in a typical permit include stating the biochemical oxygen demand, concentration of total suspended solids, total nitrogen in a water sample, and flow monitoring of the effluent via an acceptable measurement device. For water, the permits are very broad and have different requirements based on the types and sources of discharges. All of these regulations would affect the team's process design because the start up costs to build a green field process includes the permits and fees. All of this must be included in the economic analysis as part of the land costs and necessary yearly fees. Also, these regulations would classify as a constraint because the waste to fuel plant must be designed on paper and on ChemCAD to meet the regulations of the government, or else it is not a feasible process to pursue.

VI. Background Skills

The previous coursework that has applied to this project includes the courses of Process Design, Reactor Design, Principles of Chemical Engineering, Separations, and Process Safety. Principles of Chemical Engineering applied through the extensive mass balances helped determine the inputs and outputs of the process as well as the conversions of intermediates. These balances were important because they provided necessary information to input into ChemCAD in order to simulate the process. The coursework in Process Design provided many useful methods to build the ChemCAD simulation,

determine sizing for the reactors, provide the overall economic analysis through CapCost, and increase the process efficiency. Important equations used from this course were the economies of scale equation to determine the cost when scaling up the process, shown in **Equation 1**.

$$Cost_{new} = Cost_0 * \left[\frac{Stream\ Size_{new}}{Stream\ Size_0} \right]^n \quad (1)$$

Equation 1: Scale up formula for unit operations

Reactor Design coursework contributed to determining designs of the HTC and FT reactors, their sizing, and the rate of reactions for conversion of the feed to the product. The design equation for a batch reactor was used, shown in **Equation 2**, to find the conversion time for a certain input and rate constant.

$$\frac{dX}{dt} = \frac{-r_A V}{N_{A0}} \quad (2)$$

Equation 2: Design equation for batch reactor

The rate of reaction inside the FT reactor had its own rate equation with the addition of an iron catalyst, shown in **Equation 3**⁹. This equation was used to figure out the equilibrium constant for the water-gas shift reaction.

$$K_P = e^{0.31688 + 4.1778 \cdot z + 0.63508 \cdot z^2 - 0.29353 \cdot z^3} \quad (3)$$

Equation 3: Equilibrium equation inside FT reactor with iron catalyst

Separations was useful in the many separating units added to the design to remove acidic gases, tars, pollutants, and carbon dioxide from the system to input the right H_2/CO ratio into the FT reactor. The syngas cleaning steps in the process simulation require many separation concepts to know what kind of separators to input into the ChemCAD. Finally, the coursework in Process Safety helped the team to do a large HAZOP “what if” analysis of the entire process and consider all dangers that the process has when operating. Each unit operation was considered in its own hazard assessment to ensure that all safety considerations are met.

VII. Literature Review

To successfully design this process, a lot of research had to be done to understand two of its different aspects: HTC and diesel production. For diesel production using syngas, literature had a well developed process for which not a lot of changes are required. Our sources mainly consisted of a report by the National Renewable Energy Laboratory (NREL). The report helped the team understand the process of diesel production and what parameters were needed to produce it. The NREL report was mainly used as a reference on the syngas cleaning process and FT reactor parameters, so everything before that was excluded from being considered. The report helped with understanding the mass balance around the FT reactor by using known relationships such as the Anderson-Schulz-Flory³. For the syngas cleaning the team used a similar process to the one in the report using a direct contact quench and a wet scrubber along with an absorption column that uses monoethanolamine to absorb all the sour gases such as CO_2 and H_2S . Although the NREL report helped with the design of the process some things

were different and had to be changed due to the use of an iron catalyst instead of a cobalt catalyst. Articles such as “Techno-economic analysis of production of Fischer-Tropsch liquids via biomass gasification: The effects of Fischer-Tropsch catalysts and natural gas co-feeding”¹⁰ helped with calculating and understanding the kinetics of the FT reactor. The other aspect of literature review was related to the HTC reactor and gasifier. For the HTC reactor, research on the composition of the food waste and hydrochar was needed to understand what the gasifier would produce. Research by The University of Nevada, Reno specifically Dr. Charles Coronella, helped get an understanding of the overall HTC process and how it turns waste into fuel. The research also helped with the overall design of the HTC reactor. Research such as “Hydrothermal carbonization of food waste: simplified process simulation model based on experimental results”¹¹ helped with the mass balance of the HTC reactor as it helped understand the composition of the components of the process. For the gasifier “Thermochemical Biomass Gasification: A Review of the Current Status of the Technology.”¹² along with other papers helped understand how the gasifier works and how to balance it, since it is one of the most complicated mass balances of the entire process. Overall Literature and previous research helped immensely in the design of the process as there were well known standards for certain process and a lot of research for the new technology that differentiates the designed process from what is known.

VIII. Input/output Design

The basic input/output diagram of this process is given in **Figure 7**.

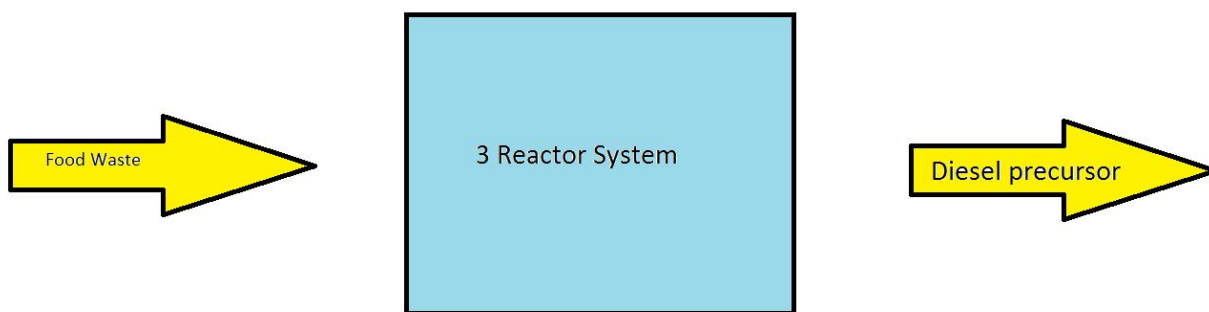


Figure 7: Simplistic in/out diagram showing feedstock and overall product

Preliminary Economic Analysis

Using the initial mass balance on the system, and ignoring all other costs, a level 0 economic assessment is initially assembled. For 1 metric ton of food waste being processed per hour, the most conservative estimate is that the organic waste will be free of cost and that ultra low sulfur diesel, expected to be produced from the FT synthesis, would sell at the wholesale price of \$2.21/gallon.¹³ Assuming that the diesel will have a density of 0.832 kg/L, 1584 gallons of diesel will be produced each day. Assuming a single pass conversion of 100% conversion in the FT reactor about 250kg of diesel precursor is formed per hour. This translates to \$1,278,000 per year. From a level 0 analysis the process is profitable. Additional revenue streams may come from a tipping fee and selling CO₂ produced during the process. The economic analysis section of this report goes into much greater detail to determine a much more profitable feed rate.

System Single-Pass Mass Balance

Table 1 shows the dry basis weight percent of carbon, hydrogen, oxygen, nitrogen, and sulfur making up the food waste as well as the hydrochar based on data collected from “Hydrothermal carbonization of food waste: simplified process simulation model based on experimental results”¹¹. These calculations were based on a 1 ton feed of dry food waste.

Table 1: Weight percent of each element in the food waste as well as the hydrochar

Element/ Molecule	Food waste (wt%) (1 ton)	Hydrochar (wt%) (750kg)
C	53.9	64.9
H	3.02	2.98
N	7.56	7.95
S	0.6	0.5
O	34.9	23.6

At 200°C, the solid yield from the HTC reactor is 75%. So 75% of the food waste is converted into hydrochar at this temperature. 2.5 times the dry weight of the food waste of water is added to the HTC reactor along with the food waste. The other 25% of the solids making up the food waste exit the HTC as waste water (71.2% of the water initially added to the HTC as well as any water generated by the HTC reaction) , exit gas

(CO₂ and CO), and some of the waste water (28.8% of the water initially added to the HTC) is combined with the hydrochar product stream to help it flow into the gasifier.

Table 2 shows the concentration of elements in the waste water, **Table 3** shows the amount of carbon dioxide and carbon monoxide that leaves as gas. **Table 4** shows a water balance on the entire system based on 1 ton of dry food waste.

Table 2: The concentrations of various elements in the wastewater of the HTC process

Element/ Molecule	Concentration in wastewater (kg element/ kg H ₂ O)
C	0.010
H	N/A
N	0.006
S	0.001
O	0.02

Table 3: weight percent of carbon in initial food waste leaving system as gas.

Gas	(wt% of initial carbon in feed)
CO ₂	4.25
CO	0.32

Table 4: Water balance throughout the entire system

Location	HTC Feed	Generate d in HTC	HTC waste	Gasifier Feed	Gasifier Exit	Added to FT feed	Generate d in FT
Water flow (kg)	2500	72	1852	720	0	78	185

Table 4 summarized the overall system, making it easier to understand what is going on. 2.5 tons of water are initially added to the HTC reactor for the reaction to proceed and possibly help the food waste to flow more easily. Then the HTC reaction generates 72 kg of water. 1852 kg of water leaves the system for waste treatment, but 720 kg flows the hydrochar into the gasifier. The water is gasified as well in order to increase the hydrogen ratio of the syngas. That is why no water is left exiting the gasifier. 78 kg of water is added to the FT feed in order to facilitate the water gas shift reaction in the iron catalyst FT reactor which is explained in further detail in the next section. Finally 184.7 kg of water is created during FT synthesis.

A volume percent table of syngas exiting a typical entrained flow reactor was used to assume that there was three times as much CO in the syngas as CO₂.¹⁴ Since 99% of the carbon reacts in the gasifier a rough and simplified reaction shown in equation 4 was

made to show what is occurring in the gasifier. **Table 5** shows the amounts of gas created in the gasifier in terms of mass with the basis of 1 ton of dry food waste entering the HTC. The impurities include trace amounts of ash, nitrogen, and sulfur which may have made it into the syngas. The ash/slag is where the majority of the sulfur, nitrogen, and unreacted carbon from the hydrochar go after gasification.



Equation 4: Gasifier reaction

Table 5: Mass balance on gasifier (1 ton HTC food waste feed basis)

Component	Amount (kg)
CO	840.3
CO ₂	440.1
H ₂	102.8
Ash/Slag	67.6
Impurities	19.2

An estimate of 54% single pass carbon monoxide conversion is assumed to give an estimate of the amount of waxes that can be sold to refineries for hydrocracking and diesel creation. This mass balance was used as a basis to create the Chemcad simulation which was first generated without recycle streams in order to simplify the process. So for

now, only the single pass is taken into account. In order to make the process more clear, **Table 6** shows the components leaving the gasifier and undergoing a water gas shift reaction before the FT process, even though the water gas shift reaction occurs within the FT reactor. **Table 7** details the Fischer Tropsch mass balance assuming the water gas shift reaction occurs first.

Table 6: Water gas shift reaction balance on syngas components

Element/ Molecule	Entering WGS(kg)	Leaving WGS (kg)
CO	840.3	718.5
H ₂	102.8	111.5
CO ₂	440.1	631.54
H ₂ O	78.3	0

Table 7: FT synthesis reaction mass balance

Element/ Molecule	Entering FT(kg)	Leaving FT (kg)
CO	718.5	431.1
H ₂	111.5	68.3
CO ₂	631.54	631.5
H ₂ O	0	184.7
Wax	0	144.8

As can be seen by the huge amounts of H₂ and CO left over after FT synthesis a recycle will need to be added in order to get the most value out of the product. Here the wax is simplified as one single carbon and hydrogen compound, but the actual range of compounds created by FT synthesis is a huge. Further details on the composition of the FT reactor products and the recycle stream added to the chemcad simulation are detailed in the detailed technical design subsection of this report.

One thing to note is that these values found here for the mass balances match the ones calculated by ChemCAD. The main differences arise from the recycle stream that was introduced in the simulation and some miscellaneous water amounts that were tracked

more closely in chemCAD. An example of additional water amounts that are present in ChemCAD come from the additional water added to the absorber with the cleanup through the amine solution.

IX. Summary of Design/Innovation

The design of the process is based on the well known production of diesel from syngas. Normally the process involves some carbon rich material being gasified to produce a synthesis gas, or in the case of the NREL³ report corn stover, which is a biomass. The team designed a unique process with food waste as the feedstock of choice. Since food waste was used as a biomass rather than grinding and burning the corn stover as in the NREL³ report the designed process used a HTC reactor. The HTC process will bring unique characteristics to the rest of the process due to the low sulfur amount in the resulting biochar according to the HTC research of Dr. Charles Coronella. The team designed the process to have two batch reactors so that one can be running while the other one goes through the process of heating, emptying, and preparing for the following batch. Both of the reactors will feed into a pressurized vessel that will ensure a continuous feed for the rest of the process. After the Vessel a gasifier will produce syngas and will remove a certain amount of solids from the process. Since the team decided on a high temperature gasifier there will be less solid contaminants and tars to clog up the process as stated in the NREL report. Following the gasifier a direct quench unit will cool down the process and remove any solids left in the stream, then a wet scrubber will remove any other smaller solids within the stream. Once the stream is cooled down, it will be fed to an absorption column that will remove gases such as NH₃,

CO₂ and H₂S using monoethanolamine (MEA). The syngas cleaning method up to this point was followed from the NREL³ report. The differences came with the use of an iron catalyst in the FT reactor. Since the iron catalyst is not as sensitive as the cobalt catalyst a sour water gas shift reactor was not needed before the gas cleaning to reach the desirable literature ratio of H₂ to CO of 2.1. Instead, the iron catalyst will have a water gas shift reaction as a side reaction. This was done to remove a unit of operation to reduce the cost of the process. Although cheaper, the quality of the products is not as great as if the cobalt catalyst was used. An overall comparison that further asserted the choice of iron vs cobalt is found in **Figure 8**.

CATALYST COMPARISON - PERCEPTION vs. REALITY				
Concept	Perception		Reality	
	Co	Fe	Co	Fe
Chain Growth Probability (α)	High	Low	Intermediate	Low to High
Activity	High	Low	High	High
Olefin Selectivity	Low	High	Low	High
H ₂ /CO Ratio for Feed	2+	0.5 to 2.5	1.0 to 2+	0.5 to 2+
Water-Gas-Shift, Activity and CO ₂ Selectivity	Very Low	High	Very Low	Intermediate to High
Methane Selectivity	High	Low	Intermediate	Low to very low
Temperature	Only Low	Low to High	Only Low	Low to High
Temperature Sensitivity, Activation Energy	Very Sensitive	Slight	Slight	Slight
Temperature Sensitivity, Product Distribution	Sensitive	Slight	Very Sensitive	Very Slight
Pressure Sensitivity, Product Distribution	Very	Slight	Very	Slight
Sulfur Tolerance	Very Little	Very Little	Very Little	Intermediate
Stability, Life Time	Long	Short	Long	Long
Cost	Expensive	Cheap	Expensive	Cheap to Expensive
Separation from Wax	Easy	Difficult	Easy	Very Difficult
Robustness	Excellent	Poor	Excellent	Very Poor

Figure 8¹⁵: Detailed comparison of cobalt vs iron catalysts for FT chemistry.

Another unit that was removed was the Zinc Oxide guard bed, which was used to clean the syngas and reduce the concentration of H_2S and other damaging gases to parts per billion. This is not necessary for an iron catalyst as it can withstand higher H_2S concentration. The syngas will react to create various chains of hydrocarbons, according to the Anderson-Schulz-Flory Relationship as shown in the NREL report. The FT produced favorable chains for diesel production that would then be sold wholesale.

X. Detailed Technical Design

Overview

Figure 9 shows the overall PFD for the process that the team designed. Since the overall process has a large amount of streams and unit operations, the process will be broken up into four sections for stream and unit op analysis.

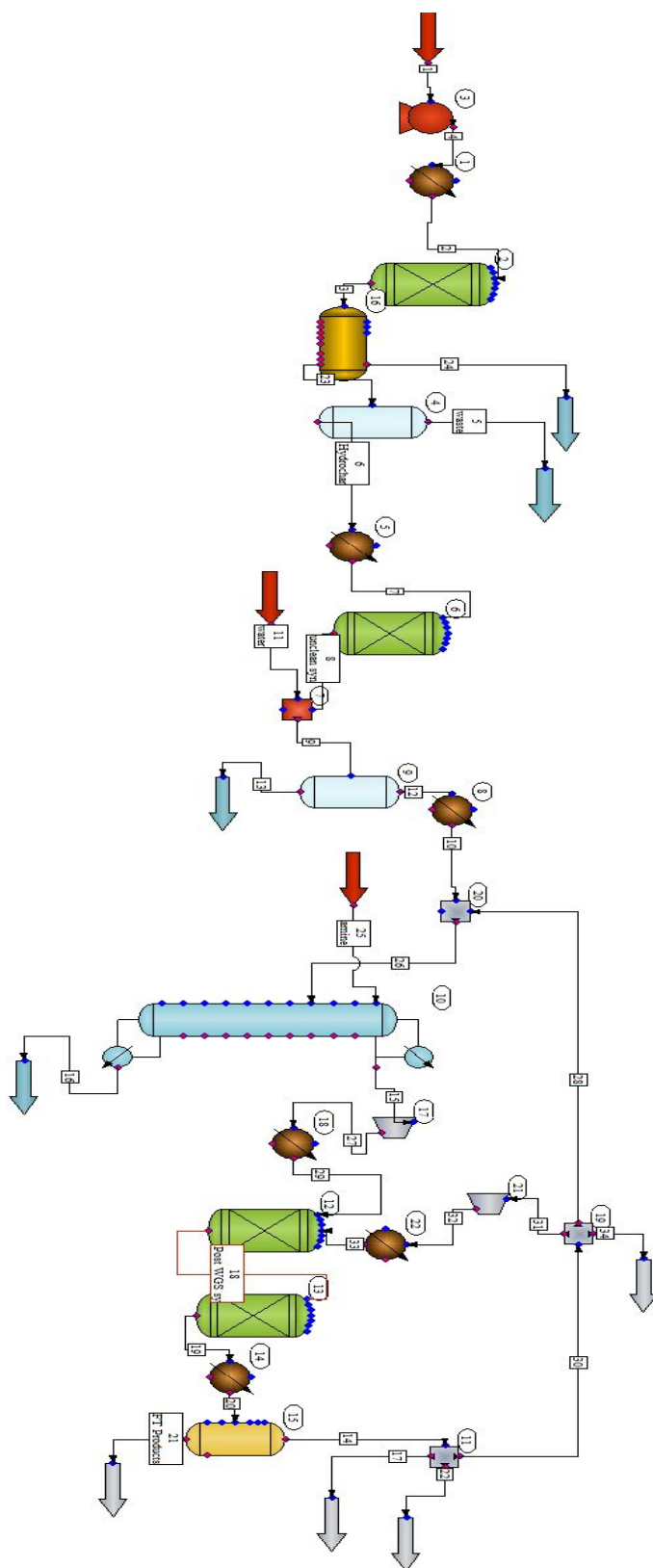


Figure 9: ChemCAD flowsheet of the overall process.

HTC reactor system

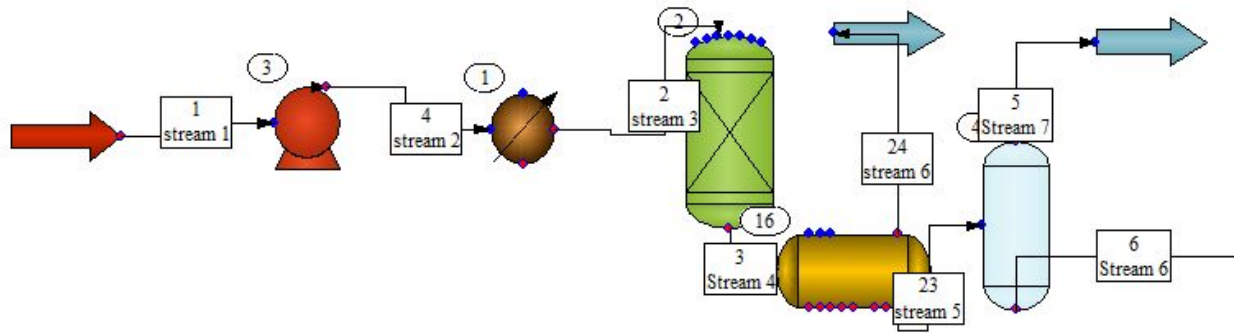


Figure 10: The HTC reactor portion of the chemcad simulation.

Feedstock Assumptions:

A pilot scale plant was assumed for this process with 1000 kilograms of food waste processed per hour. The choice of food waste itself was an economic decision. A discussion with Fulcrum Biofuels taught the team that separation of organic waste from other waste once it is in a landfill is not a trivial matter. A significant amount of extra labor would be needed in order to pull waste from a landfill rather than a more purified food waste feed acquired from grocery stores, restaurants, universities, and hospitals. Both a worst case scenario and a best case scenario was assumed to economically analyze this pilot scale model to determine whether there was any chance it could be economically viable with this small feed rate.

Food waste and hydrochar both had to be input into chemcad in order to create somewhat valid thermodynamic values (heat of reaction and heat duty) for the process. Both food waste and hydrochar were assumed to have a boiling point similar to that of carbon (5000 degrees Celsius)¹⁶ due to their high carbon content.

Food waste was assumed to have the same heat capacity and enthalpy of formation as cellulose since they are both complex carbohydrates. This heat capacity is 1.5KJ/kgK.¹⁶ The heat of formation of food waste was assumed to be -5KJ/g.¹⁷ Hydrochar was assumed to have the same heat capacity and enthalpy of formation as lignite since they are both carbonaceous fuels. The specific heat of the hydrochar is 1.45 KJ/KgK.¹⁸ The enthalpy of formation of the hydrochar is assumed to be -2.5KJ/g.¹⁹

Hydrothermal Carbonization reactor assumptions

Figure 10 shows a single HTC reactor, but in reality the HTC reactor section of the plant will be run with two autoclave batch reactors. The heat exchanger and pump in **Figure 10** shown before the HTC reactor will not actually be present in the system they were input into chemcad to prepare the simulation's feed to the desired temperature and pressure.

The team assumed that the high pressure built up in the HTC reactor would allow the rest of the process to occur without any need for pumps. This assumption was made based on the lack of pumps in the NREL simulation the project is based on as well as the continuously decreasing pressure noted after the HTC part of the process.

The batch HTC reactor assumption was also made in order to remove the need for a pump capable of pushing solid waste into a high pressure reactor. These types of pumps do exist, but they are expensive and according to Fulcrum Biofuels this part of the

process has been a serious problem for creating a continuous process for converting food waste into diesel. The HTC reactors will be made of stainless steel due to the acidic water created during the reaction. All of the unit operations before the acid gas treatment system are made of stainless steel in order to prevent corrosion of the unit operations.

The two autoclave reactors were sized by designing them to be 80% full during operation. Each of the autoclave HTC batch reactors will need to be 1.946m³ in order to process a total of 1 metric ton of dry food waste feedstock per hour. The material was selected as stainless steel and Capcost determined the price of the reactors based on size, material, and reactor type.

Vessels:

Vessels in the system such as the storage vessel, the knockout drum, and the flash drum were all sized using a combination of engineering heuristics from Analysis, Synthesis, and Design of Chemical Processes as well as Capcost.

Post HTC storage vessel (V-101):

The storage vessel that contains the product of the HTC reactors is designed to be 85% full with 30 minutes worth of HTC product. Each batch HTC reactor has a reaction residence time of 30 minutes, so they alternate filling the storage vessel in order to keep the process semi-continuous as well as minimize any problems operators might have with loading the autoclave reactors with food waste. The maximum pressure was assumed to be 10% greater than the normal operating pressure. This drum is vertical due to its small size. The volume of this storage vessel was found to be 2.059m³. The material is stainless steel.

Knockout Drum vessel (V-102):

This drum occurs directly after the storage vessel it works as a three-phase separator.

This drum is used to separate the hydrochar slurry from extra waste water and waste gases produced during HTC such as carbon dioxide and carbon monoxide. The volume of the drum is designed to hold 10 times the the liquid volume passing through it per minute. This gives a drum volume of 0.534m^3 . The max operating pressure of this drum is 10% greater than the operating pressure. The drum is vertical due to its small size. The Length of this drum is exactly three times greater than the diameter. The material is stainless steel.

simulation in this report because its cost was estimated using **Equation 4** detailed in the Economics section. Given more time the team would have been able to estimate the size of the gasifier using reactor design equations and rate laws for the various reactions happening in the gasifier.

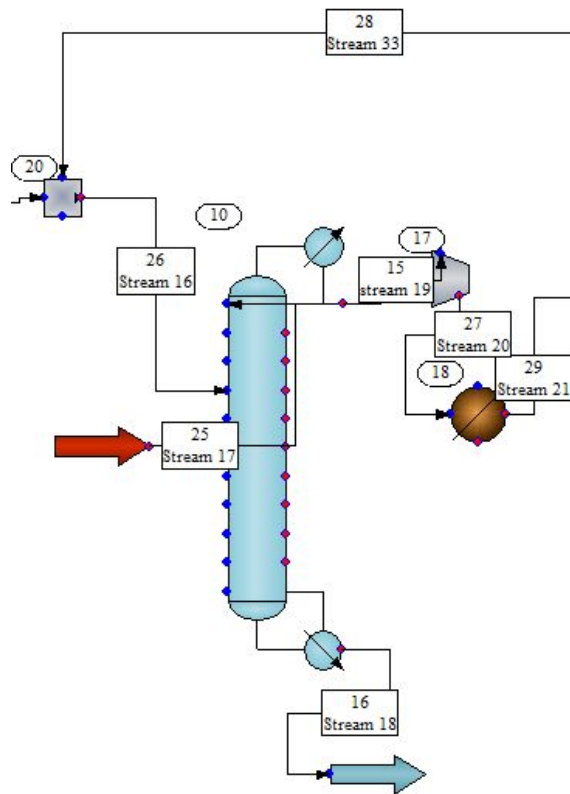


Figure 12: Acid Gas Removal System section of Chemcad simulation

Acid Gas Removal System

An absorption column with a flow of 20% monoethanolamine (MEA) flowing through it was used to clean the syngas exiting the gasifier of acidic gases (H_2S) and CO_2 . The heat exchanger and compressor are considered part of the capital cost of the acid gas removal system. The capital cost of the acid gas removal system was calculated using equation 3 from the NREL report ^[2]. Exact sizing of the compressor and the heat exchanger were not necessary for this reason. However, the heat duty of the heat exchanger and the power of the compressor given by chemcad were used to estimate utility cost of the acid gas removal system in capcost. To obtain the number of stages necessary for the absorption

column a trial and error method was used until the unit converged. Once the converging value was found, other values close to it were tested and the amount of H_2S separated was checked to pick the correct number of stages. The number of stages found was 15.

Although the absorption column correctly simulated H_2S absorption the unit was not able to correctly simulate the absorption of CO_2 . The compressor and heat exchanger are used to reach the desirable temperature and pressure to feed into the FT reactor.

Table 10: Stream Table for Acid Gas Removal System

Stream No.	28	26	25	16	15	27	29
Name	Stream 33	Stream 16	Stream 17	Stream 18	stream 19	Stream 20	Stream 21
-- Overall --							
Temp C	42.0000	40.1677	96.0000	91.4796	95.9800	111.7230	200.0000
Pres bar	23.5800	23.5800	22.7500	22.7500	22.7500	24.9700	24.9700
Vapor mole fractio	1.000	1.000	0.0000	0.0000	1.000	1.000	1.000
Molar flow kmol/h	75.0728	166.7131	1458.9399	1454.0027	171.6512	171.6512	171.6512
Mass flow kg/h	1848.2222	3243.9590	29787.3262	29714.0371	3317.2664	3317.2664	3317.2664
Flow rates in kg/h							
Water	4.6794	4.6794	24816.9219	24709.6973	111.9160	111.9160	111.9160
food waste	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
hydrochar	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Carbon Dioxide	1356.7583	1796.8583	0.0000	21.6286	1775.2295	1775.2295	1775.2295
Carbon Monoxide	385.6773	1225.9773	0.0000	1.9701	1224.0073	1224.0073	1224.0073
Hydrogen	59.1095	162.2796	0.0000	0.2901	161.9894	161.9894	161.9894
Ammonia	0.0000	2.1994	0.0000	2.1994	0.0000	0.0000	0.0000
Hydrogen Sulfide	0.0000	3.9746	0.0000	3.9746	0.0000	0.0000	0.0000
Nitrogen	14.0586	20.0516	0.0000	0.0227	20.0289	20.0289	20.0289
MDEA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.5241	0.5241	0.0000	0.0015	0.5226	0.5226	0.5226
Dimethyl	1.7755	1.7755	0.0000	0.0018	1.7736	1.7736	1.7736
Propyl hydride	0.8534	0.8534	0.0000	0.8533	0.0001	0.0001	0.0001
Isobutane	1.0705	1.0705	0.0000	1.0705	0.0000	0.0000	0.0000
2-Methylbutane	2.3086	2.3086	0.0000	2.3086	0.0000	0.0000	0.0000
Hexane	9.4898	9.4898	0.0000	0.0984	9.3914	9.3914	9.3914
Dipropylmethane	11.8265	11.8265	0.0000	0.0066	11.8199	11.8199	11.8199
N-Octane	0.0576	0.0576	0.0000	0.0576	0.0000	0.0000	0.0000
N-Nonane	0.0215	0.0215	0.0000	0.0215	0.0000	0.0000	0.0000
N-Decane	0.0077	0.0077	0.0000	0.0077	0.0000	0.0000	0.0000
Undecane	0.0027	0.0027	0.0000	0.0027	0.0000	0.0000	0.0000
Dodecane	0.0009	0.0009	0.0000	0.0009	0.0000	0.0000	0.0000
Tridecane	0.0004	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000
Tetradecane	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
N-Pentadecane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cetane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-Octadecane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-Nonadecane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-icosane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-C16-CycloC5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Heptadecane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Monoethanolamin	0.0000	0.0000	4570.4048	4569.8184	0.5873	0.5873	0.5873

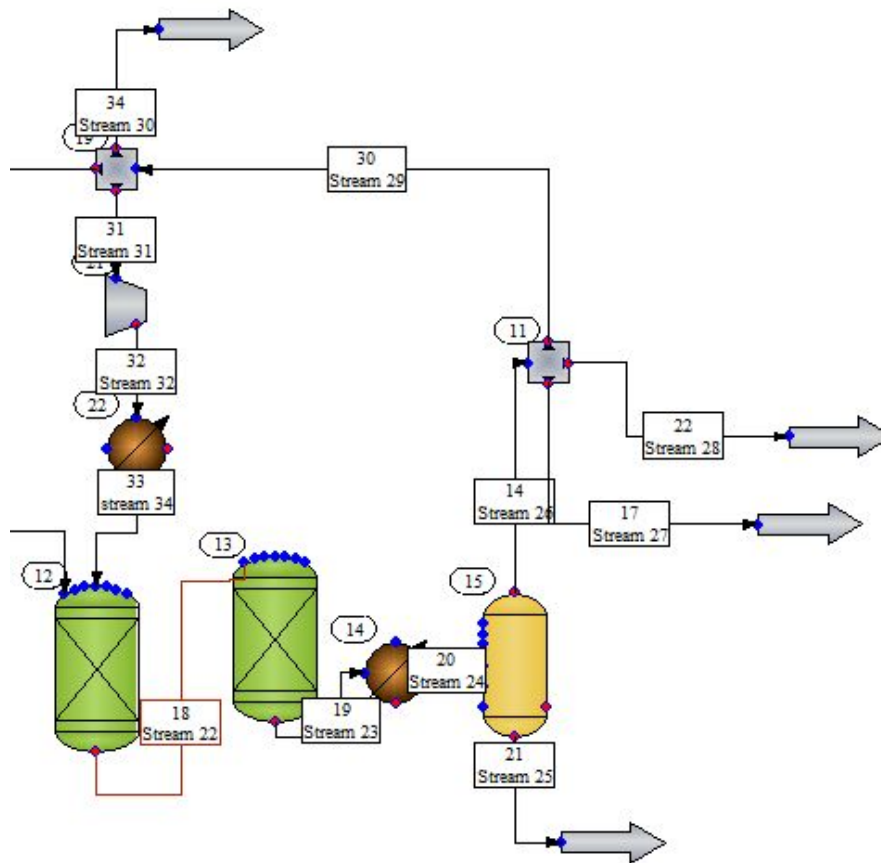


Figure 13: FT Reactor and recycle section of Chemcad simulation

FT Reactor System

To simulate the water gas shift reaction occurring in the FT reactor due to the iron catalyst, a separate reactor was used to simulate it while another reactor simulated the FT reactor. To properly simulate the FT reactor a mass balance was needed. The mass balance was found using a relationship given by the NREL report. To properly produce diesel products based on weight fraction, a chain growth factor of about 0.9 needed as seen in **Figure 14**. The chain growth factor is a function of partial pressures of CO and

H₂ along with temperature. Assuming a chain growth factor of 0.9 the mole fraction of each alkene can be found.

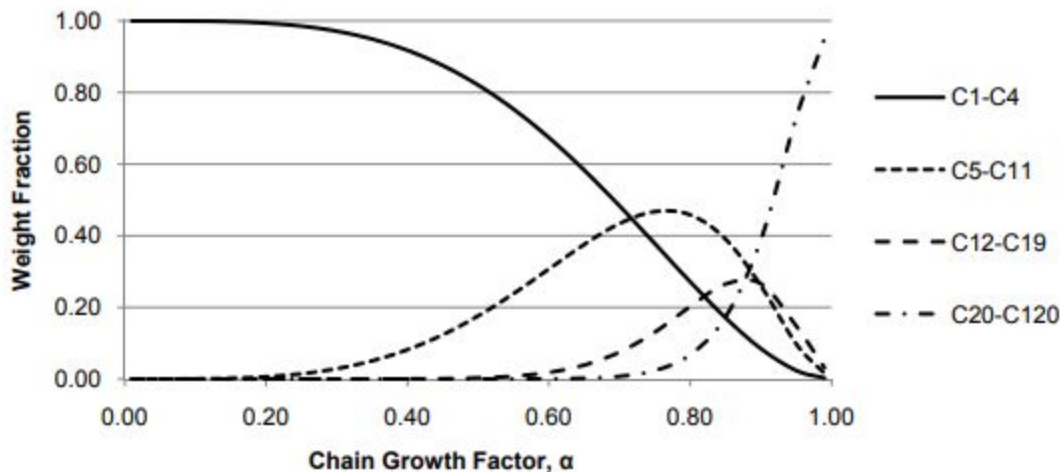


Figure 14: Weight fraction vs Chain growth factor (α)^[2]

Using Anderson-Schulz-Flory (Equation 5)³ the weight fraction of each carbon chain was found.

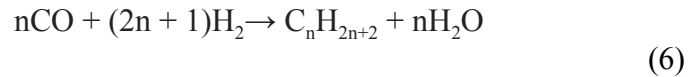
$$\text{Weight fraction}(Cx) = \alpha^{x-1} \times (1 - \alpha) \quad (5)$$

Equation 5: Weight fraction Anderson-Schulz-Flory

Where x is the number the carbon chain contains. Once each fraction is found a solve block in the NREL report was used to produce mole fractions. Where the mol fraction for every chain containing 1-20 carbons was obtained and the rest was considered waxes.

Once the mole fraction of each carbon chain was found the amount of CO and H₂ and the amount of H₂O produced was calculated. To calculate the amount of moles required it was assumed that only one mole of FT products was made. Based on the mol fractions

calculated before the amount of moles of the other reactant and products was calculated using the FT reactor reaction³ which is:



Equation 6: Chemical equation for FT reactor

Using these coefficients the **Figure 15** was made to calculate each mol fraction and adding to obtain the total amount of moles required to produce 1 mol of products.

Carbon Chain	moles produced	number of carbons in chain(n)	moles of CO needed	2n+1	moles of H2 needed	n	moles of water produced
C1	0.01	1	0.01	3	0.03	1	0.01
C2	0.018	2	0.036	5	0.09	2	0.036
C3	0.0243	3	0.0729	7	0.1701	3	0.0729
C4	0.02916	4	0.11664	9	0.26244	4	0.11664
C5	0.0328	5	0.164	11	0.3608	5	0.164
C6	0.03543	6	0.21258	13	0.46059	6	0.21258
C7	0.0372	7	0.2604	15	0.558	7	0.2604
C8	0.03826	8	0.30608	17	0.65042	8	0.30608
C9	0.03874	9	0.34866	19	0.73606	9	0.34866
C10	0.03874	10	0.3874	21	0.81354	10	0.3874
C11	0.03835	11	0.42185	23	0.88205	11	0.42185
C12	0.03766	12	0.45192	25	0.9415	12	0.45192
C13	0.03672	13	0.47736	27	0.99144	13	0.47736
C14	0.03559	14	0.49826	29	1.03211	14	0.49826
C15	0.03432	15	0.5148	31	1.06392	15	0.5148
C16	0.03294	16	0.52704	33	1.08702	16	0.52704
C17	0.0315	17	0.5355	35	1.1025	17	0.5355
C18	0.03002	18	0.54036	37	1.11074	18	0.54036
C19	0.02852	19	0.54188	39	1.11228	19	0.54188
C20	0.02702	20	0.5404	41	1.10782	20	0.5404
waxes	0.36473	21	7.65933	43	15.68339	21	7.65933
total moles	1		14.62336	483	30.24672	231	14.62336

Figure 15: Distribution and coefficients of each reaction for production of each carbon chain.

Based on the calculations the coefficients for the overall mass balance were found and used to simulate the process on chemcad. The coefficients then would yield the following equation.



Equation 7: Overall mass balance chemical equation

In the above equation the FT products has the mole fractions distribution found with Anderson-Schulz-Flory.

The resulting products from the FT reactor were then cooled down to 35 °C and then they were flashed at 42 °C to keep the desirable products in liquid form making it easier to remove methane, propane and other gases. The rest of the process was replicated from the NREL using stream splitters to recycle some products back to the FT and others back to the distillation column. The liquid products can be then sold to a refinery since the majority will be waxes that can be hydrocracked as well as low sulfur diesel.

Flash drum vessel:

This drum (V-103) is the final unit operation in the process it is used to separate the valuable high-carbon chain diesel precursors from left over syngas and nearly worthless products produced by FT chemistry such as methane. Specifications from the GPSA Engineering data book were used to size this drum.²⁰ Maximum allowable vapor velocity must be determined using the Souders Brown Equation shown in **Equation 8** in order to calculate the size of the vessel.

$$v = k \times \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (8)$$

Equation 8: Equation used to determine the maximum allowable vapor velocity of the drum.²¹

The variable k is the vapor velocity factor and it can be assumed to be 0.32 near an operating pressure of 300psig according to the GPSA Engineering data book.²⁰ ρ_L and ρ_V are density of the liquid stream leaving the drum and the density of the vapor stream leaving the drum respectively. Then the relationship in **Equation 9**, where Q is volumetric flow rate of the vapor exiting the top of the drum, v is the maximum allowable vapor velocity, and A is the cross sectional area of the drum, can be used to determine the cross sectional area of the drum.

$$Q = vA \quad (9)$$

Equation 9: Relationship between volumetric flow rate, velocity, and area.

From this cross sectional area, the diameter of the drum can be determined. From this diameter, length can be assumed to be between 3 to 5 times greater than the diameter. A factor of 3.5 was chosen to determine length. The length of the drum is 3.04m, the diameter of the drum is 0.865m. The drum is vertical and it is made of carbon steel.

Table 11: Stream Table for FT reactor system

Stream No.	18	19	20	21	14	17
Name	Stream 22	Stream 23	Stream 24	Stream 25	Stream 26	Stream 27
-- Overall --						
Temp C	200.0000	200.0000	35.0000	42.0000	42.0000	42.0000
Pres bar	24.9700	24.9700	24.8400	23.5800	23.5800	23.5800
Vapor mole fractio	0.9880	0.8781	0.8738	0.0000	1.000	1.000
Molar flow kmol/h	231.7730	190.9337	190.9337	23.8618	167.0719	1.3366
Mass flow kg/h	4797.4136	4796.5742	4796.5742	683.4160	4113.1567	32.9052
Flow rates in kg/h						
Water	49.7353	417.7786	417.7786	407.3648	10.4139	0.0833
food waste	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
hydrochar	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Carbon Dioxide	3022.8464	3022.7878	3022.7878	3.3675	3019.4202	24.1554
Carbon Monoxide	1430.3699	858.3466	858.3466	0.0345	858.3118	6.8665
Hydrogen	216.7041	131.5513	131.5513	0.0050	131.5463	1.0524
Ammonia	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen Sulfide	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nitrogen	31.2877	31.2877	31.2877	0.0009	31.2868	0.2503
MDEA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.9423	1.1663	1.1663	0.0001	1.1663	0.0093
Bimethyl	3.1955	3.9514	3.9514	0.0002	3.9512	0.0316
Propyl hydride	0.6835	2.1807	2.1807	0.2814	1.8992	0.0152
Isobutane	0.8573	3.2253	3.2253	0.8430	2.3824	0.0191
2-Methylbutane	1.8489	5.1552	5.1552	0.0174	5.1378	0.0411
Hexane	16.9912	21.2560	21.2560	0.1369	21.1191	0.1690
Dipropylmethane	21.2912	26.4976	26.4976	0.1781	26.3195	0.2106
N-Octane	0.0461	6.1519	6.1519	6.0237	0.1282	0.0010
N-Nonane	0.0172	6.9588	6.9588	6.9109	0.0479	0.0004
N-Decane	0.0062	7.7069	7.7069	7.6897	0.0172	0.0001
Undecane	0.0021	8.3768	8.3768	8.3709	0.0059	0.0000
Dodecane	0.0007	8.9627	8.9627	8.9606	0.0021	0.0000
Tridecane	0.0003	9.4584	9.4584	9.4575	0.0009	0.0000
Tetradecane	0.0001	9.8642	9.8642	9.8640	0.0002	0.0000
N-Pentadecane	0.0000	10.1848	10.1848	10.1848	0.0001	0.0000
Cetane	0.0000	10.4209	10.4209	10.4209	0.0000	0.0000
N-Octadecane	0.0000	10.6736	10.6736	10.6736	0.0000	0.0000
N-Nonadecane	0.0000	10.6991	10.6991	10.6991	0.0000	0.0000
n-Icosane	0.0000	10.6659	10.6659	10.6659	0.0000	0.0000
N-C16-CycloC5	0.0000	150.0963	150.0963	150.0963	0.0000	0.0000
Heptadecane	0.0000	10.5825	10.5825	10.5825	0.0000	0.0000
Monoethanolamin	0.5874	0.5863	0.5863	0.5862	0.0001	0.0000

Table 12: Stream table for FT reactor system

22	30	34	31	32	33
Stream 28	Stream 29	Stream 30	Stream 31	Stream 32	stream 34
42.0000	42.0000	42.0000	42.0000	49.9682	200.0000
23.5800	23.5800	23.5800	23.5800	24.9700	24.9700
1.000	1.000	1.000	1.000	1.000	0.9962
6.6829	159.0525	23.8579	60.1218	60.1218	60.1218
164.5263	3915.7261	587.3588	1480.1449	1480.1449	1480.1449
0.4166	9.9140	1.4871	3.7475	3.7475	3.7475
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
120.7768	2874.4880	431.1732	1086.5568	1086.5568	1086.5568
34.3325	817.1130	122.5670	308.8688	308.8688	308.8688
5.2619	125.2321	18.7848	47.3377	47.3377	47.3377
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.2515	29.7851	4.4678	11.2588	11.2588	11.2588
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0467	1.1103	0.1665	0.4197	0.4197	0.4197
0.1580	3.7616	0.5642	1.4219	1.4219	1.4219
0.0760	1.8081	0.2712	0.6834	0.6834	0.6834
0.0953	2.2680	0.3402	0.8573	0.8573	0.8573
0.2055	4.8912	0.7337	1.8489	1.8489	1.8489
0.8448	20.1054	3.0158	7.5998	7.5998	7.5998
1.0528	25.0562	3.7584	9.4712	9.4712	9.4712
0.0051	0.1220	0.0183	0.0461	0.0461	0.0461
0.0019	0.0456	0.0068	0.0172	0.0172	0.0172
0.0007	0.0164	0.0025	0.0062	0.0062	0.0062
0.0002	0.0057	0.0008	0.0021	0.0021	0.0021
0.0001	0.0020	0.0003	0.0007	0.0007	0.0007
0.0000	0.0008	0.0001	0.0003	0.0003	0.0003
0.0000	0.0002	0.0000	0.0001	0.0001	0.0001
0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0001	0.0000	0.0000	0.0000	0.0000

General Unit Op Sizing Assumptions

Heat Exchangers:

Heat Exchangers 101, 102, and 103 were all sized using **Equation 10**. Q_h is the heat duty which is based on the heat duty calculated in the Chemcad simulation, ΔT_{lm} is the log mean temperature difference, and U is the heat transfer coefficient which was chosen based on heat exchanger heuristics. U was equal to $60 \text{ W/m}^2\text{-K}$ for water to gas heat exchange and $850 \text{ W/m}^2\text{-K}$ for water to liquid heat exchangers.²² All heat exchangers were chosen as shell and tube heat exchangers due to their prevalence in chemical process noted from the chemcad simulations created in CHE 450. Cooling water entering the heat exchangers was assumed to be between 30 degrees celsius and 45 degrees celsius.²² Heat exchangers which will cool HTC and gasifier products will be made of stainless steel due to the acidic nature of some of the products of these reactions. Heat exchangers present after the removal of the acid gases will be made of carbon steel.

$$Q_h = U * A * \Delta T_{lm} \quad (10)$$

Equation 10: Equation used to determine the surface area of the heat exchangers in the process

Compressors:

Compressor 101 is used to increase the pressure of the recycle stream entering the FT reactor based on the NREL report recycle stream. It is considered a reciprocating compressor with 75% efficiency due to the relatively small pressure increase it is

responsible for. The cost estimate for this unit op was taken directly from cost estimates available in the chemcad simulation and input into capcost.

Unit Op Tables

Table 13: Details about heat exchangers sized using design equations.

E-101	E-102	E-103
A = 63.7m ²	A = 14m ²	A = 12.6m ²
Floating head, stainless steel, shell-and-tube design	Floating head, carbon steel, shell-and-tube design	Floating head, carbon steel, shell-and-tube design
Process stream in tube	Process stream in tube	Process stream in tube
Q = 464 MJ/h	Q = 1409 MJ/h	Q = 308 MJ/h
U = 60 W/(m ² K)	U = 850 W/(m ² K)	U = 60 W/(m ² K)
Max pressure rating = 25bar	Max pressure rating = 25bar	Max pressure rating = 25bar

Table 14: Details about Vessels sized using design equations.

V-101 (storage)	V-102 (3-phase separator)	V-103 (flash drum)
L = 1.83m	L = 2.6m	L = 3.04m
D = 0.60m	D = 1m	D = 0.865m
Vertical	Vertical	Vertical
stainless steel	stainless steel	Carbon steel
Max pressure rating = 32.7bar	Max pressure rating = 32.9bar	Max pressure rating = 25bar

Table 15: Details about reactors used in the PFD.

R-101, R-102 (HTC batch reactors have same specification)	R-103 (Gasifier)	R-104 (FT Reactor)
V = 1.95m ³	Entrained-Flow	Carbon Steel
Stainless Steel	Stainless Steel	PBR
Batch, Autoclave	High Temperature	150kg iron catalyst
Max pressure rating = 30 bar	Max pressure rating = 30 bar	Max pressure rating = 25bar

Table 16: Details about towers in the PFD

T-101 (Acid gas removal system)
15 trays, absorption column, stainless steel, max pressure = 25 bar

Table 17: Details about compressors in the PFD

C-101 (Compressor)
Carbon steel, max pressure = 25 bar, power = 58.6 MJ/h, 75% efficiency, reciprocating compressor

XI. Economic Analysis

Assumptions and Unit Op Sizing:

All unit ops besides the gasifier, quench system, acid gas absorption system, and FT reactor system were sized according to their respective sections in the detailed technical design subsection of the project. Once the size, material of construction, and type were selected these unit operations were input into Capcost and an estimate of bare module cost was returned.

Gasifier, quench, acid gas absorption column and Fischer Tropsch reactor system

The FT reactor, high temperature gasifier, direct water quench system, and the acid gas removal system were calculated based on economic data and **Equations 11** and **12** from

the NREL report the project simulation is based on. The sizing exponent (n) was given for the HT gasifier and quench system as shown in **Equation 12**, it was also given as 0.72 for the FT reactor, but for the acid gas removal system a standard value of 0.6 was assumed since none was given. This value is based on a standard value from Analysis, Synthesis, and Design of Chemical Processes.²² The NREL report also provided Stream Size₀ and Cost₀ for each unit op sized using this method. After determining the costs of these unit operations based on the equations below, they were added into capcost in order to determine their contribution to the total module cost of the process.

$$Cost_{new} = Cost_0 * \left[\frac{Stream\ Size_{new}}{Stream\ Size_0} \right]^n \quad (11)$$

Equation 11: General form of equation used to size several components in the project.³

$$Cost_{HTgasifier} = \frac{(638 \cdot 80\%)}{8} \cdot \left[\frac{2000MT}{2500MT} \right]^{0.7} \quad (12)$$

Equation 12: Example of the equation used to specify the price of a high temperature gasifier.³

Utility Assumption:

All utilities for unit operations which needed heating and cooling utilities (HTC reactors, gasifier, acid gas removal system, heat exchanger) were calculated based on heat duties

from chemcad. All cooling utilities used cooling water and all heating utilities used high pressure steam. These utilities were selected in capcost and calculated by capcost.

Electricity is needed for the compressor that is in the recycle stream as well as the compressor that is part of the acid gas removal system. The prices of this electricity was taken as \$0.06/kWh and input into capcost based on the hourly power load in chemcad.²²

Waste Treatment Assumptions

A small amount of very clean flue gas leaves the system (CO_2 , CO , H_2) with trace amounts of contaminants. This clean flue gas can be released directly to the atmosphere since it has all been through an acid gas removal process. There is a large amount of waste water in this process which will be treated with secondary (filtration + activated sludge) for \$43/1000m³.²² This price was calculated and input into Capcost so it can contribute to the total cost of manufacturing.

Raw Material cost:

The feedstock material for this process will not cost anything which is beneficial for the process, however the amine solution (MEA) used in the acid gas removal system will have a significant cost. MEA is assumed to have a wholesale cost of \$1875.²³ Luckily MEA can be regenerated. MEA is regenerated with a very high yield in the NREL report, but there is no specifics about how much needs to be purchased annually. Therefore it is assumed that 24 times the hourly feed of MEA will be purchased each year. MEA was used because it is the solvent that was used to clean acidic gases such as H_2S from the syngas in the NREL report.

Equation 13 and **Equation 14** were used to determine the molar flow rates of MEA and water used in the pilot plant process. These Equations are shown below.

$$\dot{M}_{MEA} = (\dot{M}_{CO_2,syn} + \dot{M}_{CO_2,rec} + \dot{M}_{H_2S,syn})/0.35 \quad (13)$$

Equation 13: Used to determine molar flow rate of MEA needed to remove acid gases from syngas.³

$$\dot{M}_{H_2O} = \frac{\dot{M}_{MEA} * MW_{MEA}/0.20}{MW_{H_2O}} \quad (14)$$

Equation 14: This equation was used to figure out the amount of water needed to dilute the MEA to 20%.³

According to the NREL report cobalt catalyst for FT synthesis is \$64 per pound. Since iron catalyst is up to 230 times cheaper than cobalt its price is nearly negligible within the context of the process.²⁴ Since the amount of iron need in a pilot scale FT reactor would only be 300lb and would need to be changed once every two years its cost was ignored in these economic estimations.

Economic assumptions:

Most of the assumptions used for calculation of capital costs are based on the same assumptions made in the NREL report so a direct comparison can be made.

Tax rate: The tax rate will differ based on worst-case and best-case scenarios. For the best case scenario the tax rate will be the national average for chemical manufacturing

26.69%²⁵. For the worst case scenario the tax rate will be 39% as it is in the NREL report.

Interest: The capcost assumed interest rate of 10% will be

Depreciation: Seven year straight line depreciation will be assumed. This is assumed in the NREL report and was a common assumption in CHE 450.

Operator pay: Operator pay will be based on the national mean which is \$24.62 hourly.²⁶

Working Capital: Working capital will be 15% of the fixed capital investment.³

Land cost: The land cost will be 6% of the total purchased equipment cost.³

Diesel cost: The diesel cost for the worst case scenario is based on the current wholesale price of ultra-low-sulfur diesel on the west coast. This price is \$2.21 per gallon.²⁷ The

\$3.75/ gallon of wholesale diesel is an idealized price based on overcoming the COM_d.

Cost Evaluation

Using the methods detailed for each unit op in the assumption section, sizing and other relevant info was input into Capcost software. Bare module costs were calculated for two different pilot scale scenarios using Capcost software. Table 18 details the difference between the two scenarios. The total module cost factor in Capcost is by default 1.18 and the grass roots factor is 0.5.

Pilot Scale Plant (Worst Case Scenario)

Table 18: This table shows the differences between the worst-case and best-case scenarios for the plant.

Parameter	Best-case scenario	Worst-case scenario
Wholesale diesel price	\$3.75/gal	\$2.21/gal
Tipping Fee	\$50/ metric ton	None
FT Reactor Conversion	90%	40%
Tax rate	26.69%	39%

Material Name	Classification	Price (\$/kg)	Flowrate (kg/h)	Annual Cost
diesel	Product	\$ (0.70)	232.52	\$ (1,358,392)
MEA	Raw Material	\$ 1.88	14.00	\$ 218,453

Figure 16: Diesel product revenue and MEA raw material cost for worst case scenario.

Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
E-101	Floating Head	25	25	Stainless Steel / Carbon Steel	63.7	\$ 32,300	\$ 159,000
E-102	Floating Head	25	25	Carbon Steel / Carbon Steel	14	\$ 28,200	\$ 97,300
E-103	Floating Head	25	25	Carbon Steel / Carbon Steel	12.6	\$ 28,600	\$ 98,700

Reactors	Type	Volume (cubic meters)	Purchased Equipment Cost	Bare Module Cost
R-101	Autoclave	1.95	\$ 66,200	\$ 265,000
R-102	Autoclave	1.95	\$ 66,300	\$ 265,000

Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
V-101	Vertical	1.83	0.609	Stainles Steel		32.7	\$ 3,620	\$ 58,600
V-102	Vertical	2.6	1	Stainles Steel		32.9	\$ 6,640	\$ 156,000
V-103	Vertical	3.04	0.865	Carbon Steel		25	\$ 6,200	\$ 43,800

Added Equipment	Description	BMF ₀	Actual BMF	Purchased Equipment Cost	Bare Module Cost
Z-101	gasifier	1	1	\$ 2,523,000	\$ 2,523,000
Z-102	FT reactor	1	1	\$ 841,800	\$ 841,800
Z-103	Acid Gas Removal system	1	1	\$ 213,100	\$ 213,100
Z-104	compressor	1.3	1.29999948359644	\$ 38,729	\$ 50,348
Total Bare Module Cost					\$ 4,721,300

Figure 17: Total Bare module cost for the unit operations in the chemcad simulation in the best case and worst case scenario.

Table 19: Summary of capital costs for both best and worst case scenarios.

Total Bare Module Cost	Total Module Cost	Grass Roots Cost
\$4,721,300	\$5,620,000	\$7,670,000

Economic Options

Cost of Land	\$	337,200
Taxation Rate		39%
Annual Interest Rate		10%
Salvage Value		0
Working Capital	\$	1,151,000
FCIL	\$	7,670,000
Total Module Factor		1.18
Grass Roots Factor		0.50

Economic Information Calculated From Given Information

Revenue From Sales	\$	1,358,392
C_{RM} (Raw Materials Costs)	\$	218,453
C_{UT} (Cost of Utilities)	\$	1,090,000
C_{WT} (Waste Treatment Costs)	\$	12,720
C_{OL} (Cost of Operating Labor)	\$	102,418

Factors Used in Calculation of Cost of Manufacturing (COM_d)

$$Comd = 0.18*FCIL + 2.76*COL + 1.23*(CUT + CWT + CRM)$$

Multiplying factor for FCIL		0.18
Multiplying factor for C_{OL}		2.76
Facotrs for C_{UT} , C_{WT} , and C_{RM}		1.23
COM_d	\$	3,288,316

Figure 18: Parameters and operating costs for worst case scenario system.

Utility Used	Efficiency	Actual Usage	Annual Utility Cost
Cooling Water		464 MJ/h	\$ 1,370
Cooling Water		551 MJ/h	\$ 1,620
High-Pressure Steam		308 MJ/h	\$ 45,370
High-Pressure Steam		2160 MJ/h	\$ 318,400
NA			
NA			
NA			
NA			
High-Pressure Steam		4390 MJ/h	\$ 646,600
Unspecified			
High-Pressure Steam		498 MJ/h	\$ 73,400
Custom		58.6 MJ/h	\$ 8,134
			\$ 1,090,000

Figure 19: Utility costs for the unit operations of the process.

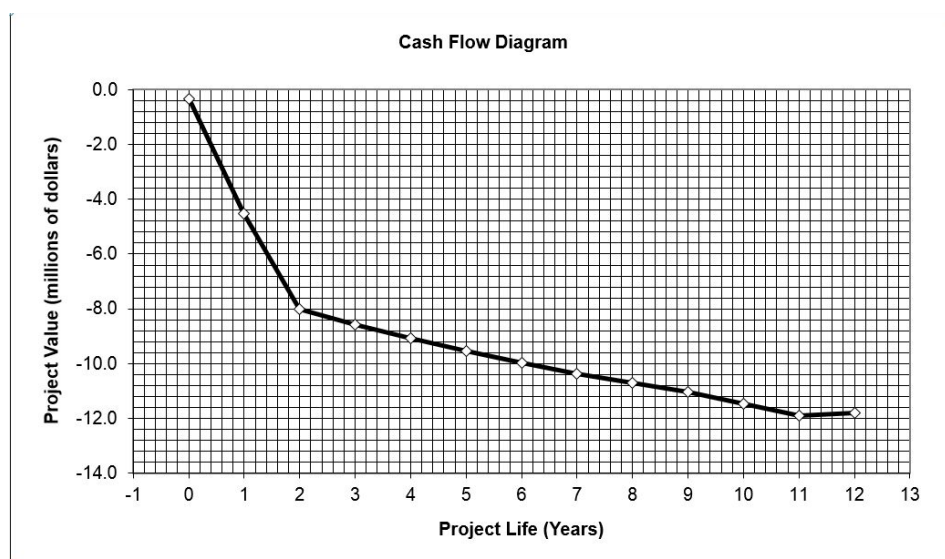


Figure 20: Discounted Cash flow diagram for worst case scenario pilot plant.

Worst Case Scenario Pilot Summary: The worst-case scenario pilot plant is not economically viable. The cost of manufacturing far outweighs the revenue made in the process so the cash flow diagram never has a positive slope. There is no payback period because it will continue losing money endlessly.

Pilot Plant (Best Case Scenario):

Material Name	Classification	Price (\$/kg)	Flowrate (kg/h)	Annual Cost
diesel	Product	\$ (1.20)	294.73	\$ (2,943,292)
MEA	Raw Material	\$ 1.88	14.00	\$ 218,453
food waste	Product	\$ (0.05)	1000.00	\$ (416,100)

Figure 21: Diesel and food waste revenue as well as MEA cost for best case scenario.

Economic Options

Cost of Land	\$	337,200
Taxation Rate		27%
Annual Interest Rate		10%
Salvage Value		0
Working Capital	\$	1,150,000
FCI _L	\$	7,670,000
Total Module Factor		1.18
Grass Roots Factor		0.50

Figure 22: Economic parameters for best-case scenario

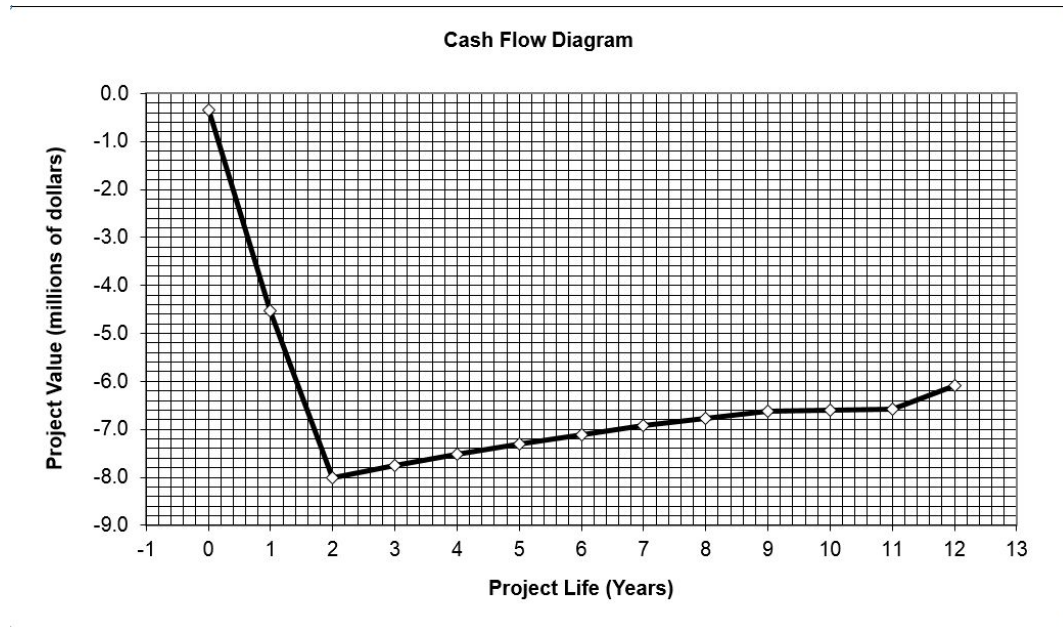


Figure 23: Discounted Cash flow diagram for best case scenario.

Best Case Scenario Pilot Summary: The best case scenario performs significantly better than the worst-case scenario but it is still not a viable plant. There would eventually be a payback period, but it would be a lot longer than even a 20 year project life. The NPV's are also still negative for the best case scenario.

Uncertainties:

All of the bare module costs that were calculated directly from capcost are based on equipment cost data that is already present in capcost. An example would be the two batch HTC reactors which were priced as autoclaves in capcost because that was the closest estimate. This is most likely not a perfect representation of a hydrothermal carbonization reactor. The prices of the gasifier, FT reactor, quench system, and acid gas

removal system are based on the NREL report from 2010. It is possible that prices may have shifted significantly in the nine years since that paper was published.

The amount of MEA needed annually for this process is a huge uncertainty and it could make or break the process. The capital cost of equipment that is needed to regenerate the MEA is also not included in these calculations, but it could become the largest economic portion of the process. The NREL report shows MEA being regenerated with negligible losses which means a small amount could last an entire year as is assumed in these calculations, but if a larger amount of MEA is needed it threatens the profitability of the process even on an industrial scale. On the opposite hand the amount of MEA needed for the process may be overestimated. The MEA gas is supposed to scrub H_2S and CO_2 out of the syngas. However, only the H_2S was removed while nearly all the CO_2 stayed in the FT feed in the team's simulation which may be due to an error in the chemcad. This leads to a large amount of CO_2 in the system since it does not react in the FT reactor. In a real system there should only be trace amount of CO_2 in the recycle stream, the actual amount of MEA should only consider the CO_2 in the syngas directly after the gasifier, the trace amount in the recycle, and the H_2S in the syngas directly after the gasifier.

Finally it is worth noting that retail and wholesale costs of diesel shift on a weekly basis. The amount of money made will change week to week based on these prices. In order to build a realistic plant of this nature, it would be wise to study diesel prices in previous years to see if there is any common patterns that result in a large rise or fall in the wholesale price of diesel.

Cost Reduction and Economies of Scale

There are several areas in which cost could be reduced for the overall process, but the pilot plant will most likely never be economically viable due to how capital cost intensive it is. This type of pilot plant could be built as a proof of concept in order to justify plans for a larger plant. The diesel being created is a commodity product, therefore large amounts need to be made in order to become profitable.⁸ This section will focus on some changes which could be made to make any size of this plant become more profitable.

There will also be capital cost and operation cost calculations for a plant processing 100 metric tons of food waste per hour, this plant will be processing 100 times more food waste than the pilot plant analyzed previously.

Utility Cost Reduction Strategies

Gasifier and HTC: The gasifier and HTC reactor make up around 90% of the utility cost as seen in **Figure 19**. This cost could be significantly reduced if a fired heater using coal, petroleum, or natural gas was used instead of high pressure steam. The capital cost would be increased from the use of a fired heater, but the utility cost reduction would make up for this. According to the cost of manufacturing equation in **Figure 18** the capital costs are only factored in the COM_D by 0.18, but the utility costs are factored in by 1.23. The environmental cost of adding fired heaters should also be taken into account. In the short term these fossil fuel utilities will certainly make the process more profitable. However, as the threat of climate change looms emission standards can become much stricter. A detailed study would need to be done to compare the cash flow to the cost of extra carbon produced and the possible fines violating emissions standards could yield.

Acid gas absorption system: The MEA is not too expensive with the assumption that only a small amount will be needed each year because it can be regenerated. However, it is possible that it is too difficult to create an amine regeneration system capable of regeneration with negligible degradation. The capital cost of the MEA regeneration system is not considered in the calculation in this report, but they could also significantly decrease the profitability of this process. Using a different solvent to remove acid gases and carbon dioxide could decrease raw material and capital costs. Aqueous ammonia is less than one third the price of MEA²⁸ and it is more environmentally friendly. Ammonia production uses only 27% of the total energy needed to create MEA.²⁹ A value added product could be created in the formation of ammonium bicarbonate and other ammonia salts after flue gas cleaning. If needed aqueous ammonia could be regenerated in a manner similar to that of MEA. MEA was chosen because it was used in the NREL report, but there are several alternatives that warrant further inspection.

Heat recycle: All three reaction in this process are highly exothermic. It may be possible to take advantage of the heat energy, especially from the gasifier, to heat up the feed to the FT reactor. The heat from the gasifier could also be used to heat the light key syngas feed coming out of the acid gas removal absorption tower. If the team had more time a more thorough energy balance would be conducted in order to make efficient use of all heat in the process in order to further reduce utility costs. The chemcad would also be updated with these energy recycles.

Capital and Operating Costs of an Industrial Scale Plant

A rough estimation of the capital and operating costs of an industrial scale plant can be conducted by applying **Equation 3** to the gross roots and total module costs shown for the pilot plant shown in **Table 2**. The sizing exponent (n) will be assumed to be 0.6 since that is the default value. The utility, labor, and waste treatment costs will be assumed to scale linearly with the capital costs. The amount of diesel produced and the amount of MEA used will scale linearly with the new food waste feed of 100 tons per hour. Land fees and working capital fees will be calculated from these assumed values. A cash flow diagram, NPV, PBP, and IRR will be calculated for the same worst case and best case scenario plants from the pilot plant analysis.

Material Name	Classification	Price (\$/kg)	Flowrate (kg/h)	Annual Cost
diesel	Product	\$ (0.70)	23252.00	\$ (135,452,201)
MEA	Raw Material	\$ 1.88	1400.00	\$ 21,845,250

Figure 24: Raw materials and products in the worst case industrial plant

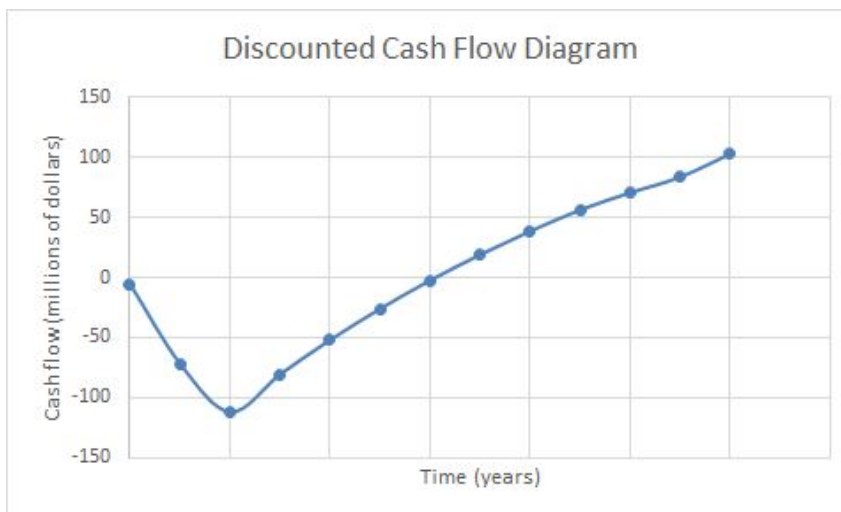


Figure 25: Discounted cash flow diagram for worst case scenario industrial plant

Material Name	Classification	Price (\$/kg)	Flowrate (kg/h)	Annual Cost
diesel	Product	\$ (1.20)	29473000.00	\$ (294,329,167,200)
MEA	Raw Material	\$ 1.88	1400.00	\$ 21,845,250
food waste	Product	\$ (0.05)	100000.00	\$ (41,610,000)

Figure 26: Raw materials and products in the best case industrial scale scenario.

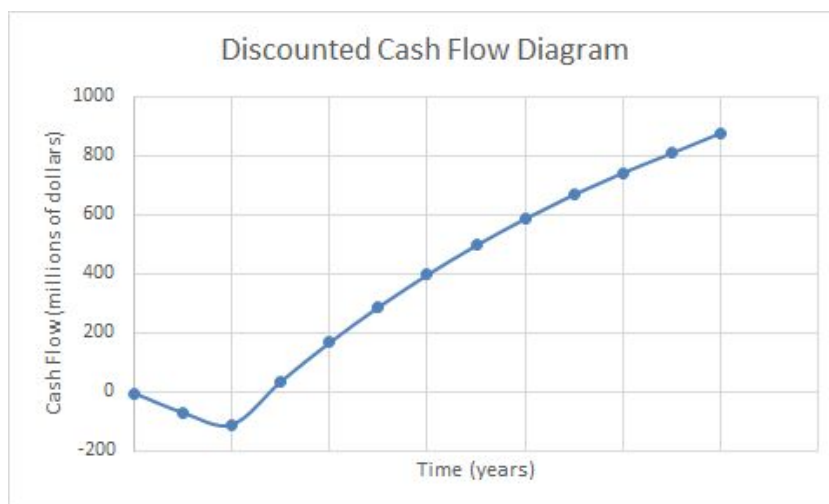


Figure 27: Discounted cash flow diagram for best case scenario industrial plant.

Even though this is only a rough estimate of the cash flow at a larger scale, it still clearly shows that the scale of this operation matters. Commodity chemicals needs to be produced at large scales in order to be profitable. **Table 20** below shows that each industrial scale scenario yielded a favorable NPV, PBP, and IRR. Since this is a best-case and worst-case scenario the truth is likely somewhere in the middle.

Profitability

The industrial scale plant clearly performs better in all categories. The industrial worst case scenario seems to be the most realistic model of a plant as it has a reasonable PBP, NPV, and IRR. The best case scenario is certainly too good to be true. In this section uncertainties such as interest rate, MEA flow rate, and tax rate will be tested via one factor at a time testing. This type of sensitivity analysis will be used to test the effect a change on one variable will have on the NPV of the entire system while all other variables are held constant. The worst-case scenario parameters will be used in this sensitivity analysis since that has yielded the most realistic looking CFD and profitability measures.

Table 20: Comparison of profitability measures.

Profitability	Pilot worst scenario	Pilot best scenario	Industrial worst scenario	Industrial best scenario
Discounted NPV (millions of dollars)	-11.8	-6.1	103	877
Non-discounted NPV (millions of dollars)	-16.5	-5.1	300	1826
Discounted PBP (years)	N/A	N/A	4	1
Non-discounted PBP (years)	N/A	N/A	3	1
IRR	N/A	-10%	25%	93%

Tax rate: Both tax rates which were used in this simulation will be tested while everything else is held constant. The effect on the NPV of the system will detail how important this parameter is to the overall calculations. **Table 21** demonstrates that a lower tax rate creates a far more profitable process as expected. The average tax rate on chemical manufacturing in 2019 is far more favorable than the one used in the NREI report in 2010.

Table 21: Sensitivity Analysis of Tax rate

Tax rate	Interest rate	Reactor Conversion	MEA flow rate (kg/h)	Discounted NPV (millions of dollars)
27%	10%	40%	1400	134
39%	10%	40%	1400	103

Interest Rate: Interest rates of 10, 20, and 30 percent will be tested while all other variables are held constant. The effect on the NPV of the system will detail how important this parameter is to the overall calculations. **Table 5** demonstrates that a larger interest rate significantly decreases the profitability of the process. A 30% interest rate even makes the NPV negative. It is important that a company running this type of operation finds investors with low interest rates on their loans.

Table 22: Sensitivity Analysis of interest rate

Tax rate	Interest rate	Reactor Conversion	MEA flow rate (kg/h)	Discounted NPV (millions of dollars)
39%	10%	40%	1400	103
39%	20%	40%	1400	23
39%	30%	40%	1400	-15

MEA Flowrate: The MEA flow rate was a huge source of uncertainty for these calculations. It is difficult to determine what the actual regeneration capabilities of a plant would be. A sensitivity analysis will be conducted to compare the assumption of 24 times the hourly flow of MEA purchased per year to a less capable regeneration system which causes the plant to purchase 24 times the flow of MEA per month. **Table 23** shows that this will be a very important point that warrants further investigation if a real project were to be designed. MEA is expensive and if the plant is not capable of regeneration without significant degradation another solvent to clean the syngas will need to be found.

Table 23: Sensitivity Analysis of MEA flowrate

Tax rate	Interest rate	Reactor Conversion	MEA flow rate (kg/h)	Discounted NPV (millions of dollars)
39%	10%	40%	16300	-5
39%	10%	40%	1400	103

Of the three parameters which underwent sensitivity analysis tax rate is the most stable. Fluctuations in the amount of MEA needed or the interest rate on the loan could make or break a project. This is suggested by the negative values for NPV which were calculated for high interest rates and high MEA flow rates. Even if the tax rate is to change significantly it is unlikely to make the process unfavorable.

XII. HAZOP Analysis

Table 24: Hazop Analysis on the HTC process.

Guide Word	Deviation	Cause	Consequence	Action
No	Temperature control	Broken sensor	Runaway reaction, explosion	Open pressure valve and shut down system
	Flow out	Blockage (tar) in waste line, Stuck Valve	Buildup in reactor, No release of gas combustion products-explosion	Interlock a flow sensor with the process. Shut down pumps and flow.
More of	Higher temperature	More energy input	Reactor overheats	Increase coolant flow rate to the reactor.
	Higher pressure	Blockage in waste line	Buildup in reactor, Explosion	Pressure relief system in reactor
Less of	Lower temperature	Less energy input	No carbonization, Poor products	Decrease coolant flow rate to the reactor
	Lower pressure	Burst line, low temperature	No carbonization, Poor products	Low pressure alarm
More than	Excess water in slurry	Variable feedstock	Undesired ratio composition of products	Composition sensor, use purified feed
Other than	Impurities in slurry	Variable feedstock	Buildup and excess waste	Composition sensor, use purified feed

Table 25: Hazop Analysis on the Gasifier process.

Guide Word	Deviation	Cause	Consequence	Action
No	Flow in	Blockage due to slurry	Undesired product Pressure build up	Shut down unit. Install flow sensor and pressure relief system for pipe.
	Flow out	Blockage due to slurry	Pressure build up explosion	Shut down unit Install pressure relief system and pressure sensors.
	Oxygen flow	Stuck Valve, blockage in pipe	Undesired product, no reactions	Shut down unit. Oxygen sensor
More of	Higher temperature	Excess feed of biochar	Runaway reaction Explosion, harm to operators	I ncrease syngas cooling in water quench
	Higher pressure	Blockage in lines, excess recycle input	Buildup in gasifier, runaway reaction, explosion	Pressure relief system in gasifier
Less of	Lower temperature	Not enough oxygen for reaction	No gases produced, excess slag, clog gasifier	Temperature sensor, control water quench
	Lower Pressure	Burst line, low temperatures	No gases produced Potential damage to the unit.	Shutdown unit Check for any tars or leftover unwanted products in the unit.
More than	Excess water in hydrochar	Excess water from HTC, faulty filter	Undesired product formation like sulfur compounds	Composition sensor, ensure output of HTC has desired composition
Other than	Leakages and air penetration during fuel feeding	Burst line, improper fuel feeding, faulty inlet equipment	Explosions, CO and particulate matter exposure, environmental pollution	Air analyzer, monitor leakages around gasifier

Table 26: Hazop Analysis on the FT reactor process.

Guide Word	Deviation	Cause	Consequence	Action
No	Cooling	Broken cooling valve	Temp increase in reactor, runaway reaction	Install high temperature alarm, emergency release valve
	Flow	Blockage in input or output	Syngas buildup and hydrocarbon buildup	Shut down unit Instal pressure relief system and pressure sensors
More of	Higher temperature	Excess feed, increase in reaction kinetics	Faster reaction, higher conversion rate, different undesired hydrocarbons, explosion	Temperature sensor, increase coolant flow, emergency cooling quench system
	Higher pressure	Blockage in lines, waste line	Buildup in reactor, runaway reaction, explosion, catalyst deactivation, coke formation	Pressure relief system in reactor
Less of	Lower temperature	Not enough heating provided to the reactor	Blockages, Unwanted products Potential damage to the unit	Ensure proper temperature monitoring on the unit.
	Lower pressure	Leaks Low temperature	Undesired products Potential damage to the unit	Pressure sensor, low pressure alarm
More than	Contamination into feed	Issues in separator, filter, or wet scrubber after gasifier	Sulfur compounds can affect, poison, or degrade catalyst. Low reactivity	Composition sensor, emergency relief valve to redirect flow from entering reactor
Other than	Catalyst poisoning	Excess contaminants (sulfur) in	Low reactivity, unreacted inputs, excess tar	Purify sungas, know life of catalyst, store excess catalyst for future use

		syngas	formation	
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XIII. References

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