Addis Ababa University

Addis Ababa Institute of Technology

School of Chemical and Bioengineering

SUGARCANE BAGASSE-BASED BIOETHANOL PRODUCING BIOREFINERY PLANT SIMULATION AND TECHNO-ECONOMIC ANALYSIS

Master's Degree Thesis Manuscript

A Thesis Submitted to the Graduate Studies of Addis Ababa University in Partial Fulfillment for Masters of Science in Biochemical Engineering

Berhe Tekle Adhanom: methiopia2@gmail.com (0914202788)

This is to certify that the thesis prepared by Berhe Tekle Adhanom, entitled ‘ sugarcane bagasse-based bioethanol producing biorefinery plant simulation and technoeconomic analysis’ satisfays the requirement for the degree of master of science (Chemical and Bio-Engineering) complies with the regulations of the university and meets the accepted standards with respect to originality and quality.

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1. Chairperson:		
2. Advisor: Dr. Ing. Hundessa Desalegn		
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DECLARATION

I, Berhe Tekle declares that this thesis, entitled as “sugarcane bagasse-based bioethanol producing biorefinery plant simulation and technoeconomic analysis”, which is prepared for master’s degree of Addis Ababa University is my original work and as far as I know, it has not been presented for the award of similar degree in any other training institutes and universities. Moreover, all the sources of materials used to do this master’s thesis have been duly acknowledged.

Name	*Date*	*Signiture*
Berhe Tekle		
Submission Date		
Advisor: Dr. Ing. Hundessa Dessalegn		

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ABSTRACT

Energy has been the driving force for economic development. However, the source of energy has become a big issue concerning the environmental pollution. Cellulosic bioethanol is one of the different types of alternative energy sources so far innovated. It is promised to replace the liquid fossil fuel and settle the fuel vs food competition. This area attracts researchers from around the world due to its abundant resource and environmentally friendly production process. Depending on that premises, this simulation-based bioethanol production research paper was dealt to investigate some of the scale up problems and to study the economic feasibility. The research paper carefully simulates the production process and analysis its techno-economic. The conceptual model used on this paper encompasses feedstock handling, pretreatment, saccharification, cofermentation, and production recovery. To validate the equation used by Aspen Plus to simulate enzyme kinetics, the mathematical equation for enzyme kinetics of hydrolysis and cofermentation were tested in Matlab. The techno-economic analysis for the overall production process was then studied depending on two models. The two models were bioethanol plant gate price assessment model (BPAM) and feedstock cost estimation model (FCEM). During the process sensitivity analysis is also performed using Aspen Plus built-in single objective function. The result of the sensitivity analysis showed that, the conversion rate of cellulose to glucose, feedstock cost, and enzyme loading have high factor in the minimum plant gate ethanol selling price determination. The relationship between scaling up and ethanol production capacity was uniformly corelated. The bioethanol for 5000 kg/h and 100000 kg/h of sugarcane bagasse was 296.518164 and 26443.563 respectively. This shows the positive correlation of the scale up and bioethanol production. In addition to that, the overall simulation result showed that the minimum plant gate ethanol selling price at breakeven point was $2.1174 per liter. This result indicates that, even in the most optimistic scenario, the price of cellulosic ethanol is much more expensive than the other similar fuels, gasoline. However, bioethanol can be competitive at some conditions. Some of the conditions that makes the biorefinery plant competitive enough on the local market are feed-in tariff and compulsory purchase of electricity, government direct subsidy, tax preference and R&D. In addition to the above condition, public awareness is also important. Finally, the researcher has recommended to government to revise the above condition to entertain such type of environmentally friendly biorefinery plants.

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ACRONYMS AND ABBREVIATIONS

BPAM	Bioethanol Plant-Gate Selling Price Assessment Model
CHP	Combined Heat and Power (Cogeneration)
DCFROR	Discount Cash Flow Rate of Return
E10	10% Ethanol Blending
FCEM	Feedstock Cost Estimation Model
FCI	Fixed capital investment
FOC	Fixed operating cost
GTP	Growth and Transformation Plan
HMF	Hydroxymethylfurfur
IRENA	International Renewable Energy Agency
IRR	Internal rate of return
ISBL	Inside-Battery-limit
MESP	Minimum Ethanol Selling Price
MGSP	Minimum Gasoline Selling Price
NPV	Net present value
NREL	National Renewable Energy Laboratory
NRTL	Non-random Two Liquid
TCD	Total Sugarcane Crushing Capacity per Day
TCI	Total Capital Investment
TEPC	Total Equipment Purchasing Cost
TPC	Total Plant Cost
VOC	Variable Operating Cost

CHAPTER 1: **INTRODUCTION**

Bioethanol has been one of the promising environmentally friendly liquid fuels. Producing bioethanol in commercial level was not as such. The main goal of this research was to digitally design economically, environmentally, and socially feasible biorefinery plant. The designing and optimization process are a process of investigation for the best way of converting sugarcane bagasse feedstock into bioethanol. Although there are ways to test the feasibility by building a pilot plant, testing by simulation was preferred for this research. Therefore, all the different possibilities will be tested and optimized by simulating the superstructure in Aspen Plus version 11. Data and information for the designing and simulation are collected from different sources. Most of sources of data and information were scientific literatures which are published in high impact journals, equipment and chemical reagent suppliers' data, the simulation software's databank, and estimation by analogies.

This research paper contains 7 chapters, which are presented in logical order. The first chapter covers all about the introduction, background of the research, objective, statement of the problem and significance of the research. Chapter two of the research covers reviewing some best literatures around the area. At this chapter theories about the bioethanol production process, steps of bioethanol production processes, inputs, and outputs of biorefinery plants, upstream and downstream technological levels and other related topics are discussed. The third chapter of this paper talks about the design basis. Two subcategories of this chapter are process conceptual modeling and simulation. At the design base, the fundamental input for the biorefinery plant were discussed. The mode, plant capacity, plant attainment, unit of measurement, type of equipment and others were selected. The fourth chapter of this research paper lists and describes about methodology of the research. The methods that are under the discussion encompasses, feedstock handling, acidic pretreatment, enzymatic hydrolysis, co-fermentation, and product recovery. The fifth chapter deals with the techno-economic analysis. Techno-economic analysis of the research concentrates on the level of technology, financial analysis, cash flow analysis and other financial statement sections. The sixth chapter talks about the result and discussion part. The result and discussion parts interpret the result of the simulation against reality. This chapter also deals with environmental impact analysis, energy integration, market assessment and others. The last

chapter of this research paper winds up and gives some policy recommendation for the government.

1.1 BACKGROUND

The world has seen an industrial revolution in between 1760 and 1840. The industrial revolution irreversibly changes the human civilization. There were so many reasons to let happen industrial revolution. Energy has been one of the key factors to let industrial revolution to happened. The economic growth of countries has been directly or indirectly related for their energy consumption. According world energy scenario analysis, the world has irreversibly changed by 4.4 folds in between 1970 and 2015(Menon and Rao 2012). During that period, the world energy demand has also increased to 2.6 folds(Coppola, Bastianoni, and Østergård 2009). However, the world economic advancement has come in the cost of the environment. This is because the source of energy for the growth was utterly dependent on natural or non-renewable energy with inefficient technologies. As a result of such utterly fossil fuel dependent economic growth, world living report (2012) shows that high developed nations have high ecological footprint and we human beings already overshoot the earth capacity. This high ecological footprint shows the negative impact of using non-renewable and non-sustainable energy. Shifting from business as usual method to more sustainable energy source has been becoming necessary. Although the grand transit movement from conventional to sustainable started earlier, progress is so slow due to some conscious resistant.

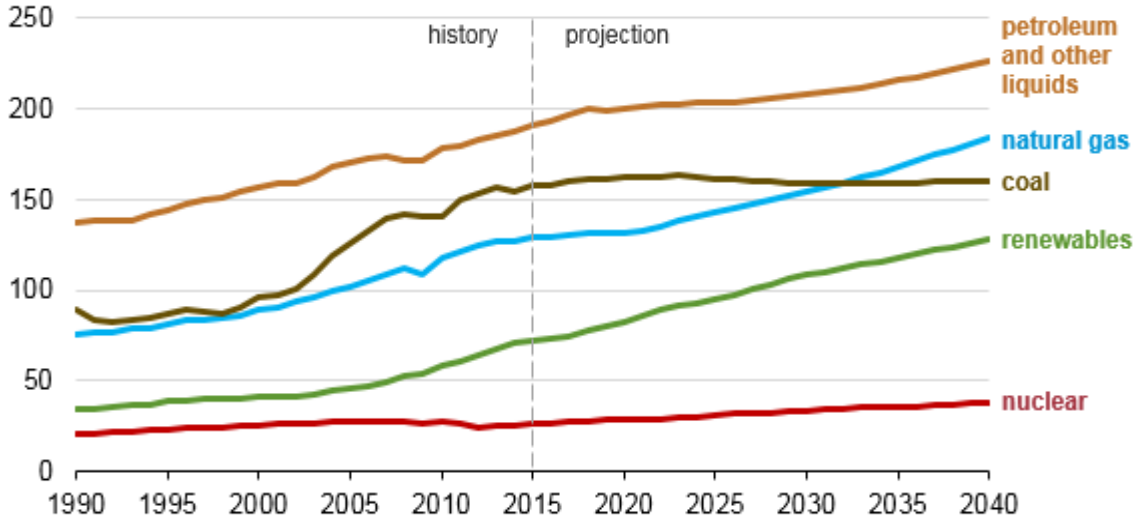


Figure 1 World energy consumption scenario by fuel source (Consumption 2015) (Tropea et al. 2014)

At this time, the technical and economic feasibility of total shift or grand transit from traditional to modern or renewable source of energy is proved possible. Currently, almost all countries (developed, developing and non-developed) have national strategic plan to transform into the renewable energy source. This is mostly come from the pressure of society and scientific community. Few of the leading nation in this grand transition movement are England, Australia, Germany, China, USA, India (IRENA, 2018). The dream for the grand transit is sustainable development and few of the frequently mentioned destinations of energy carriers are biomass, solar, wind, geothermal, hydropower. One of the most promised renewable energy sources is biomass. It has been using as source of energy even for about the whole human history as fire wood. A research also estimate that in the last 45 years, it has grown about 30 quadrillion(UN News Centre 2015).

Biofuel produces through different approaches: synthetic (gasification) and bioethanol (fermentation). The biorefinery system is based on biomass as feedstock for production of bio-based products such as biofuels and bio-chemicals. Biomass is the term used to describe all biologically produced matter using carbon, hydrogen, and oxygen. Its energy is derived from plant and animal material such as wood from natural forests, waste from agricultural and forestry processes and industrial, human, or animal wastes. The concept of a bio-based facility had been prevalent in the United States and the world in general, for hundreds of years. Paper and sugar mills are quintessential of bio-facilities where renewable feedstocks such as wood pulp and sugarcane are converted to value-added products. The use of composting facilities and waste digesters in farms and rural areas around the world has been a source of sustainable generation of electric power from renewable resources for decades. In recent times, the emphasis on biobased production using renewable resources has significantly broadened its footprint to incorporate production of fuels, power and chemicals derived from a wider variety of renewable resources (Giuliano, 2014). Some renewable transportation fuels that are already in the commercial production phase include first generation ethanol and biodiesel. The biofuels produced from renewable resources could help to reduce the world's dependence on oil and reduce CO_2 emission. These biofuels have the potential to cut CO_2 emission because the plants they are made from use CO_2 as they grow. Biomass as mentioned before includes plant materials such as trees, grasses, agricultural crops, and animal manure. Biomass formation is through photosynthesis. This is happened when solar energy is captured in the leave of plant and the energy is stored in chemical bond. The chemical equation written below shows, the carbon dioxide is fixed into

organic biomass. Then, the organic matter becomes the food for fermenting microorganism. When the cycle comes back by anthropogenic, a loop forms and the geochemical cycling continues until one of them is exempted.

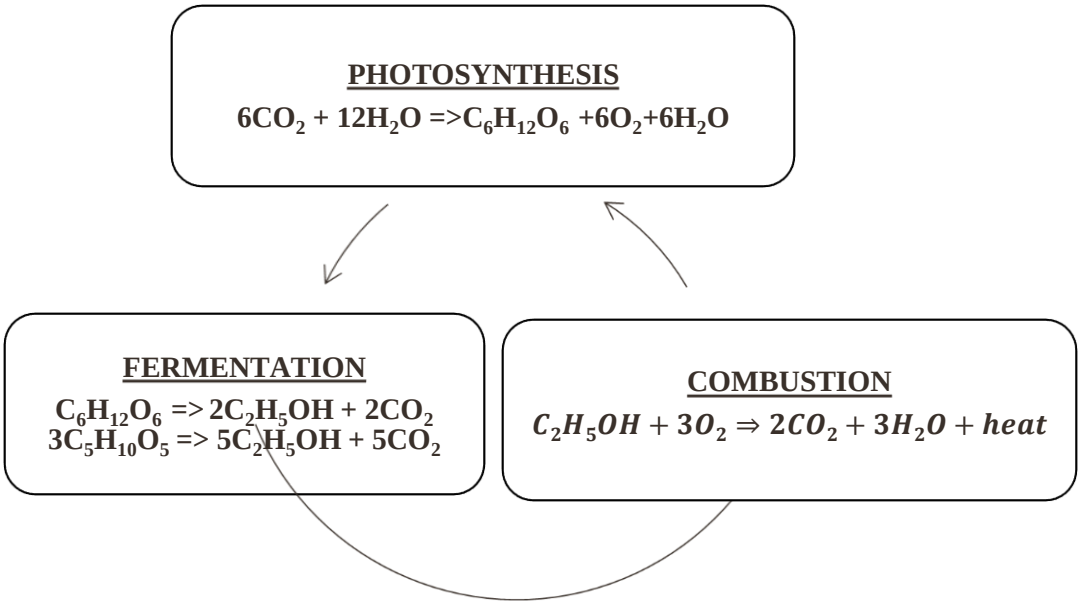


Figure 2 The cycle of energy flow connected by photosynthesis, fermentation, and combustion

Sugarcane bagasse is one of the most common biomasses, which has been treating as waste. The main components of bagasse (cellulosic) are cellulose, hemicellulose and lignin. Generally, lignocellulosic materials contain 30-50 % cellulose, 20-30% hemicellulose, and 20-30% lignin(Chang 2007). Lignin is a complex polymeric compound that helps to bind the cellulose/hemicellulose mixture; its molecular structure is very random and disorganized. Currently practiced technologies in biofuel industries are primarily based on feedstocks from food crops such as grains, sugar cane and vegetable oils. However, these processes have concern since there is a competition for their utilization in food production chains and biorefinery processes. These types of biofuel production technologies are called first-generation biofuels.

1.1.1 Generations of Ethanol as Fuel

Researchers classify thing to simplify their study. Biofuels are also classified into four generations. The generation indicates the type of source to produced ethanol.

First generation biofuel is a biofuel produced from edible crops. It is common in Brazil and United States. This stream of bioethanol production has been growing rapidly in the industrialized nations. However, it creates food versus fuel conflict. Owing to increased sugarcane production to more than offset amount of sugar diverted to ethanol production in

Brazil, this bioethanol production technology has little impact on food supplies and costs. However, in the United States, corn grain is an important food and animal feed commodity. Therefore, concerning about food supply chains and prices have been raised. The main disadvantage of first-generation biofuels is the food-versus-fuel debate. Although first generation is also common in developing country like Ethiopia from sugar molasses, food-versus-fuel conflict hinders them not invest this area. To overcome this dilemma and the overall limitation of the feedstock utilized for the first-generation biofuels, second-generation biofuels sectors are coming.

Second-generation biofuel is uncommon, but promised to lead the biofuel energy sector. The types of feedstock commonly used for second-generation biofuel are lignocellulosic waste materials, residues, and energy crops: like sugarcane bagasse. These types of biofuels have the advantage of being produced from waste materials that do not compete with the food value chains. However, the current production of second-generation biofuels is not cost effective due to the technological barriers. To overcome these problems, development and optimization demand is still required for these production technologies before their commercial production.

Third-generation Biofuel: the feedstocks for third-generation biofuel includes mainly microalgae, which produce high amounts of lipids, carbohydrates, and protein per unit of land(Giuliano, Poletto, and Barletta 2015). This type of feedstock has been considered of interest due to its fast growth rate in comparison with terrestrial plants and its versatility in terms of substrate and nutrient requirements. Microalgae and algae can grow in waste water, saline water, seawater, carbon dioxide, glycerol, and nonarable lands(Chu and Majumdar 2012). Additionally, third-generation sources have remarkable advantages such as low cost in the cultivation, high-energy production, eco-friendly, and entirely renewable. Some limitations of microalgae cultivation are low concentrations; considerable high-energy consumption due to the use of techniques such as mixing, filtration, and centrifugation; contamination problems; and low-lipid generation.

Fourth-generation Biofuel uses metabolic engineering to produce engineered algae with superior characteristics for biofuel production. Biofuel production form fourth-generation biomass may be economically viable in the long-term compared to third generation biomass. The development of cost-effective photo reactors and efficient separation technologies would decrease the capital cost significantly. The fourth-generation feedstocks include

algae(Schwab et al. 2016), industrial waste CO_2, and captured and recycled carbon are considered(Ariel, Carlos Ardona 2019). Some advantages of these feedstocks are good yields, high capacity of CO_2 capture, and high production rate. The main limitation of four-generation is related to the immaturity of the technologies(Ariel, Carlos Ardona 2019).

1.2 WHY IS BIOETHANOL USED AS FUEL?

Bioethanol is concentrated beer produced by distillation of fermented sugar. The sources are obtained from various locally available resources such as agriculture and forestry residue, dedicated starchy crops, woody and herbaceous crops, and organic portion of municipal solid waste (MSW). It has become favored due to its potential similarity on the convenient characteristics of petroleum products at competitive price(Wyman 2001). It also provides several benefits including higher engine efficiency, achieved from the high-octane number and high heat of vaporization of ethanol, and lower ozone and smog formation in its use as compared to the conventional gasoline because of its low volatility and photochemical reactivity (Dufey, 2006). Other than using the existing petroleum infrastructure, its blended use with gasoline in any proportion E5 and E10, reduces fossil fuel consumption and supply oxygen to advance further complete combustion(Van Walsum and Wheeler 2013). This reduces exhaust emission of carbon monoxide and unburned hydrocarbon without the need for engine modification (Wyman, 1996; Dufey, 2006).

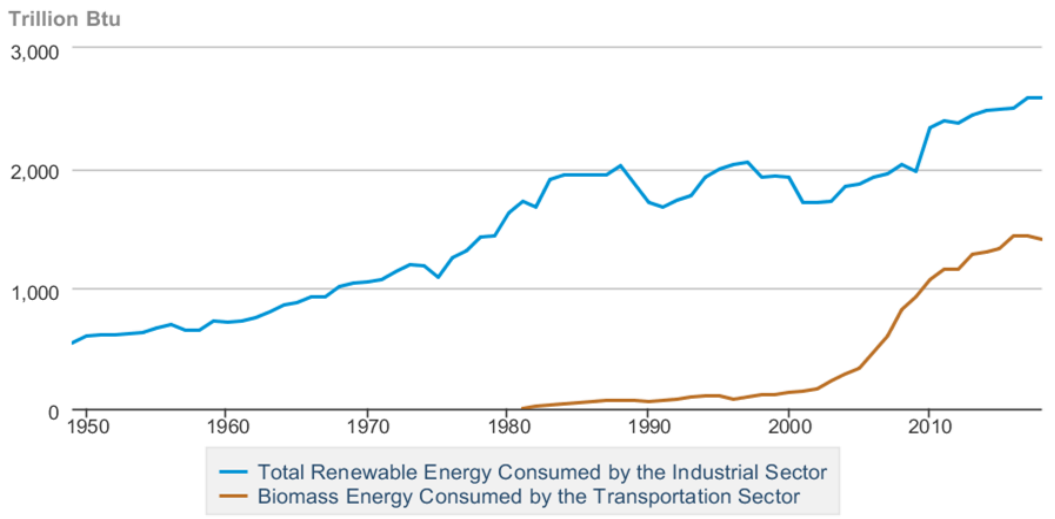


Figure 3 Renewable Energy Consumption Trends in Industries and Transportation (US.EIA, 2019)

The other greatest benefit of bioethanol lies in its potential to decrease greenhouse gas emissions through partial substitution of gasoline as a transport fuel (IEA, 2004). This could support countries to attain their commitments under the Kyoto protocol and Paris agreement

to mitigate the effects of climate change. It also decreases the burden of foreign currency outgoings for poor countries that are net importers of petroleum products and have potential to produce and use bioethanol. Other considerations following bioethanol market growth comprises the promotion of greater energy security, rural development, and poverty reduction (Dufey, 2007; Mastny, 2007).

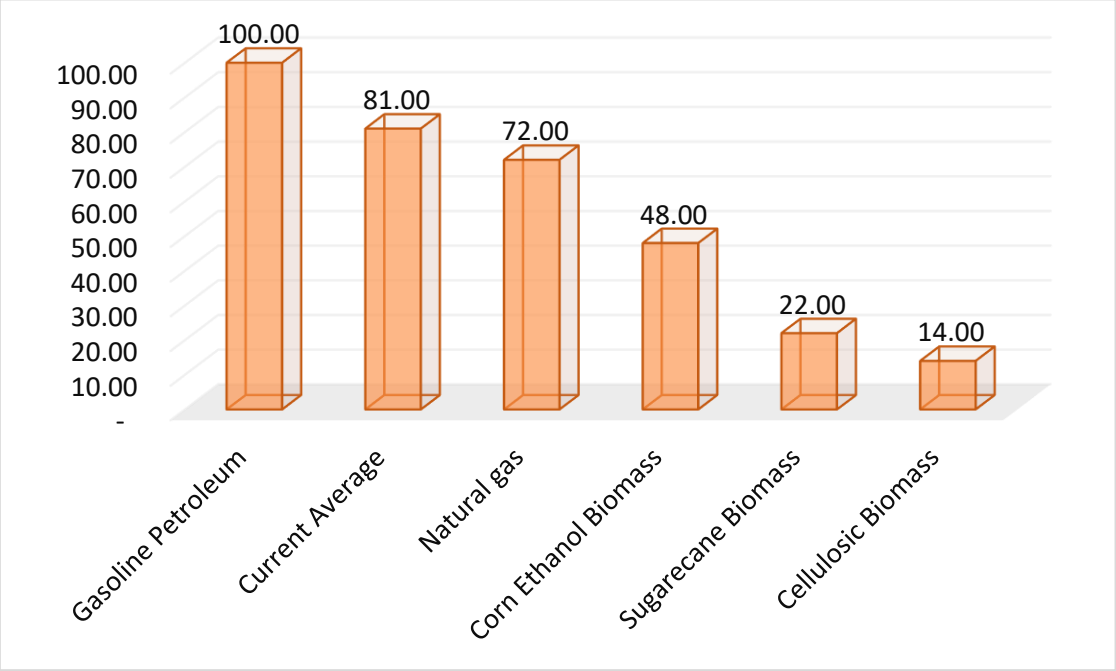


Figure 4 Percentage of carbon dioxide emission of different fuels (Huang et al. 2011)

The above bar graph shows that the status of carbon dioxide emission to the atmosphere. It indicates that using bioethanol that produced from cellulosic biomass reduces carbon dioxide emission by 85%. This also shows that bioethanol produced from cellulosic biomass (second-generation) is 7% more environmentally friendly than molasses base bioethanol (first-generation).

1.3 GLOBAL BIOETHANOL PRODUCTION STATUS

Today, bioethanol is increasing its global dominancy. Global ethanol production shows an upward trend over the last 25 years with a sharp increase from 2000. As of 2005, worldwide production capacity for bio-ethanol fuel was about 45 billion liters per year, with approximately 15% annual growth between 2000 and 2005(Kim and Dale 2004). This value increased to 49 billion liters in 2006, when the Americans produced 75% of the total world ethanol output, followed by Asia/Pacific and Europe/Africa with respective values of 15 and 10% (Talebnia, 2006). The industrial alcohol market showed a rather modest rate of growth

like the increase in gross domestic product in many countries. Like fossil fuel production, biofuel production is limited to regions by types of crop, which grow on. Production is also impacted by government subsidy and other political factors.

Table 1 Global Bioethanol Production from different feedstocks

Country	Ethanol Production (liters)	Major Feedstock
United States	40 Billion	Corn/Wheat
Brazil	25 Billion	Sugar Cane
China	3 Billion	Corn/Cassava/Rice
Canada	2 Billion	Corn/Wheat
India	1 Billion	Sugar Cane/Molasses
France	1 Billion	Wheat/Sugar Cane/Sugar Beat
Germany	750 Million	Wheat/Sugar Cane/Sugar Beat
Australia	500 Million	Sugar Cane

The market for beverage in most developed countries is stagnating due to increased health awareness. In 2009, production of fuel ethanol reached an estimated 76 billion liters, an increase of 10 percent over 2008. The United States and Brazil accounted for 88 percent of global ethanol production in 2009. Most of the increased production occurred in the United States (Talebnia, 2006). According to one estimation, U.S ethanol shows more than 360 million barrels of imported oil for gasoline production. The highest sugar prices in years, combined with adverse weather conditions in a major producing region, resulted in a drop in Brazil's ethanol production from 27.1 billion liters in 2008 to 26.3 billion liters in 2009. All ethanol produced in Brazil is from sugarcane molasses. All fueling stations in Brazil sell both pure ethanol and E25 blend. Flex-fuel cars, which can use pure ethanol, gasoline, or any blend of the two, provide the flexibility to choose fuel based on price at the pump. They have been widely embraced by drivers and represent more than 95 percent of all new cars sold in Brazil. In recent years, significant global trade in fuel ethanol has emerged, with Brazil being the leading exporter.

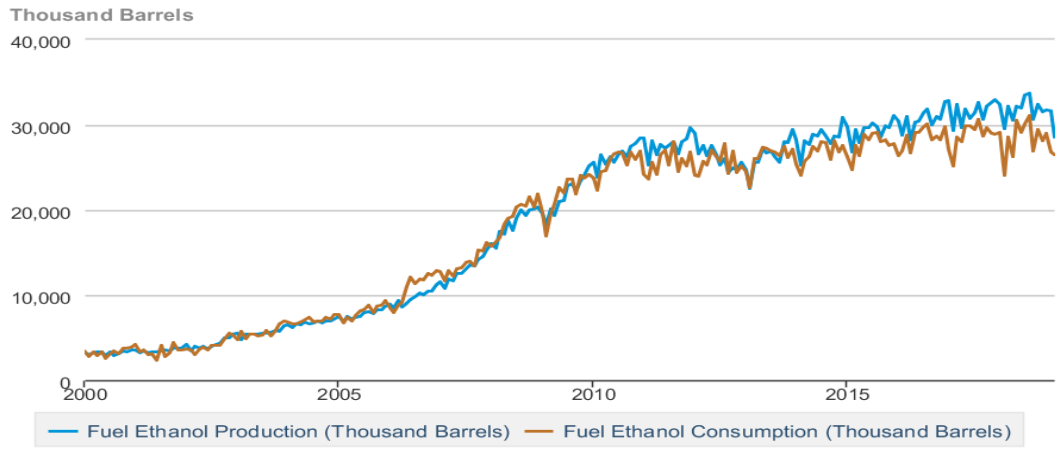


Figure 5 Worldwide fuel ethanol production and consumption trends (US. EIA, 2019)

1.4 BIOETHANOL FROM LIGNOCELLULOSE

Currently, most of the feedstocks for second-generation biofuel are treating as waste. Some of the most abundant resources in are eucalyptus tree, sugarcane bagasse, coffee husk, corn Stover, water hyacinth, agricultural waste, organic municipal waste, and others. Those can be blended and produce huge amount of second-generation biofuel. However, the target of this research paper is sugarcane bagasse-based bioethanol production. The two main advantages of producing energy from lignocellulose material are replacing fossil fuel and protecting the environment. Although ethanol production is technically feasible, economic feasibility is under investigation. Some developed countries are pushing the limit by motivating their investors. One of the most abundant feedstocks for this biorefinery plant is sugarcane bagasse. The amount of bagasse produced from each tonne of sugarcane is estimated 31%(Berhe, 2018). Most of the sugar factory cogenerates energy by burning that huge amount of sugarcane bagasse. This process of producing energy is proven inefficient. For this reason, this biorefinery plant follows the biochemical conversion method to produce liquid fuel, ethanol from sugarcane bagasse.

1.5 CHALLENGES TO PROCESS SCALE-UP

Process engineers has experience navigating a wide range of issues during pilot plant scale up. Specific types of challenges had already addressed by different researchers. Few of the most general and common challenges includes the following physical and chemical elements of a scale-up of process technology:

Reaction kinetics –In systems with good reaction kinetics, molecules from each element mix efficiently and quickly together, reaching a state of equilibrium for the solution. Various

physical and chemical factors can prevent the molecules of the mixture from mixing and colliding correctly. This can create bad reaction kinetics without proper system design.

Chemical Equilibrium: A reaction is not productive until chemical equilibrium is reached, which does not occur immediately. As increased quantities of chemicals are mixed, the time to reach equilibrium increases at a nonlinear rate.

Material properties: The properties of the materials in contact with process system chemicals are critical. Incorrectly selected materials can influence the reaction, erode over time, or make the system unnecessarily expensive.

Fluid dynamics: Keeping flow at the correct Reynolds number is important for thermal transfer and mixing efficiency. Fluid dynamics changes at a non-linear rate as systems increase in size, making changes between laminar and turbulent flow hard to predict.

Thermodynamics: Heat loss and gain can play a major role in chemical reactions. For example, some reactions discharge heat, increasing system temperature and further speeding up the reaction, letting off even more heat and causing temperatures to rise further. Controlling reaction temperature is important to a successful pilot plant scale up.

Equipment selection: The physical limitations of equipment can acutely impact the chemical reaction. Continuing the thermodynamics example, as some reactions create heat, it must escape the system in a timely matter so the reaction does not become unstable. The ratio of surface area to mixture volume determines how quickly heat can be discharged from the system. If the tank is the incorrect size, it will be difficult to control the chemical reaction, which will begin escalating quickly.

Agitation issues: Mixing techniques are crucial to achieving good reaction kinetics. As systems increase in volume, mixing presents several challenges. For example, as the volume of the reaction increases, so does the horsepower needed to stir the mixture. It is not always cost effective or feasible to add enough horsepower to stir the mixture as the system scales up. This problem is addressed by matching the tip speed of the larger agitator to the tip speed of the bench scale agitator. Creating the correct amount of turbulence within the tank to promote good reaction kinetics is an issue that is solved through angled agitators and baffles.

1.6 LIGNOCELLULOSIC BASED BIOREFINERIES

Biorefinery involves assessing and using a wide range of technologies to separate biomass into its principal constituents (carbohydrates, proteins, triglycerides, etc.), which can subsequently be transformed into value-added products in an economic, social, and environmental manner or the so-called sustainable way. The main goals of the biorefineries

are to maximize the value of the products obtained from the biomass, to increase competitiveness and prosperity of industry, to reduce fossil fuel dependency by producing the same or analogous substances demanded in the current market and to reduce the emission of greenhouse gases, and to stimulate regional and rural development. The research on utilizing renewable resources to produce non-food products has gained attention since the early 1990s. This has led to the development of new integrated processes, biomass conversion technology and biorefinery technology.

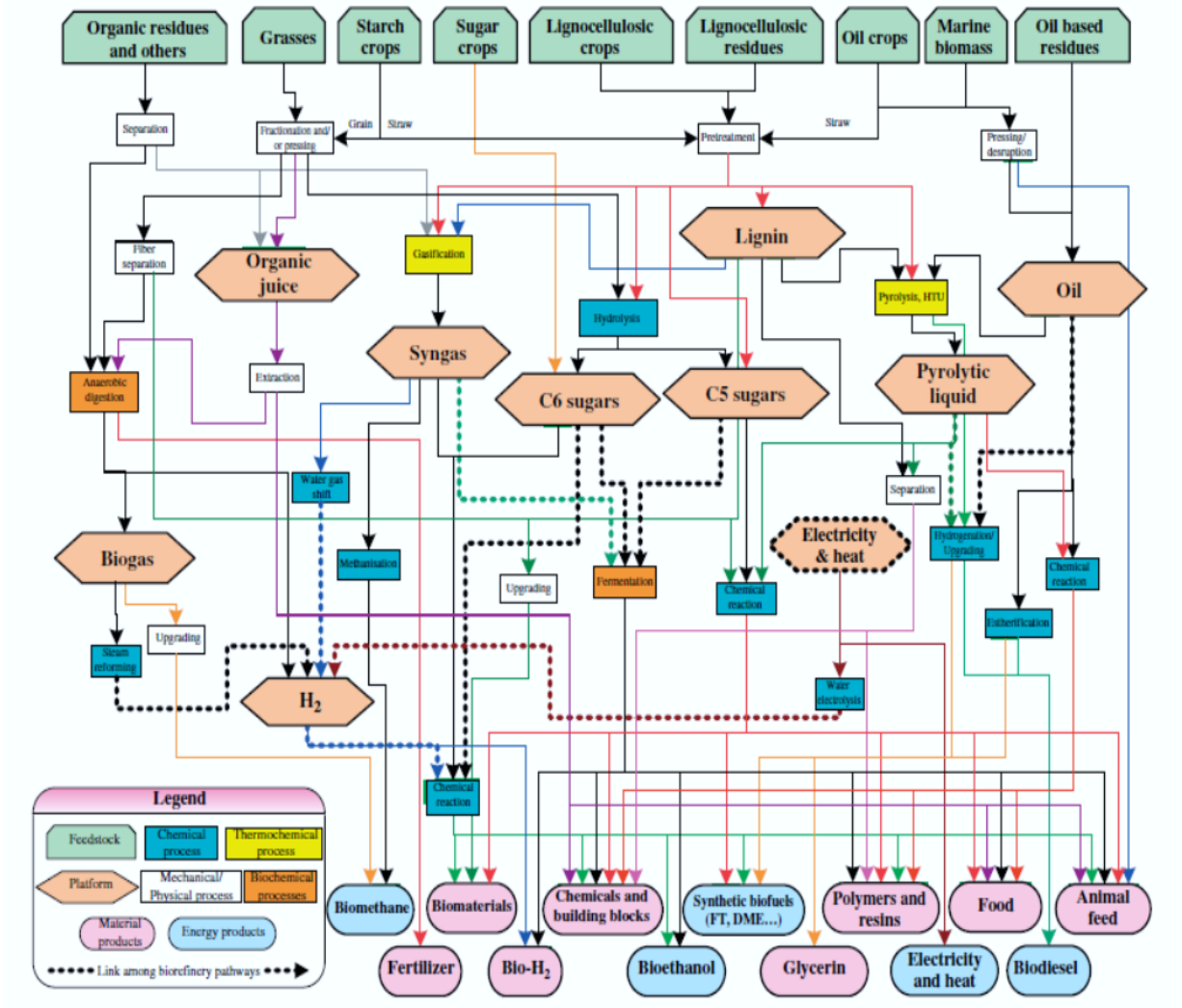


Figure 6 Network where the individual biorefinery systems are combined (Cherubini et al., 2009)

Biorefineries are categorized based on the technology adaptability towards the use of mix biomass. Based on the above criteria, biorefinery can be classified into three phases.

- Phase I: uses one feedstock to produce one specific bioproduct
- Phase II: uses one feedstock to produce multiple bioproducts
- Phase III: uses mixed feedstock to produce multiple bioproducts.

Cellulose, hemicellulose, and lignin can be used to produce the multiple products. Out of the multiple products, ethanol, which is a product of fermentation then, further processes into fuel grade. Although production of bioethanol from lignocellulosic biomass gets public attention, only few companies are fully operating. Partially implemented or pilot/commercial scale is the use of chemicals or enzymes to depolymerize the feedstock into fermentable sugars and lignin.

Table 2 Biorefinery plants from around the world

Company	**Feedstock**	**Fractionation Process**	**Scale**	**Main Product**	**Lig1nin Use**
Beta renewables (Italy)	Agricultural Residues	Steam explosion	Commercial	Bioethanol	Fuel
Abengoa Bioenergia (US)	Corn Stover, Wheat straw & Switchgrass	Steam explosion	Commercial	Bioethanol	Fuel for steam & electricity
Poet-DSM (US)	Agricultural residues	Enzymatic hydrolysis	Commercial	Bioethanol, biogas	Fuel
Abengoa Bioenergia (Spain)	Wheat straw	Steam explosion	Demo	Bioethanol	Fuel, feed additive
Chempolis (Finland)	Agricultural residues	Organosolv	Demo	Cellulose Bioethanol	Fuel
Inbicon (Denmark)	Agricultural Residues	Hydrothermal	Demo	Bioethanol	Fuel
CIMV (France)	Agricultural Residues	Organic acid and organosolv	Pilot	Cellulose, C_5 sugars, lignin	Performance materials
Biorefinery demo plant (Sweden)	Wood chips, bagasse, wheat straw, energy grass, corn stover	Dilute acid & enzymatic hydrolysis	Pilot	Bioethanol	Fuel & performance materials
Clariant (Germany)	Wheat straw	Pressurized steam treatment & enzymatic hydrolysis	Pilot	Bioethanol	fuel

1.7 PROBLEM STATEMENT

Energy has been the driving force behind every economic prosperity. However, the source of energy has also been dominated by non -renewable energy. This implies that almost every economic growth has come on the cost of the environment. Nowadays, alternative source of energy that are promised to drive the future becomes more common in the energy mix. Although they have different rate & level of development, the alternative energies include wind, solar, geothermal, biomass and others. Out of the above energy mix, biomass based liquid biofuel generation get more attention.

In this stream of liquid biofuel, there are generations. Although researchers have already confirmed the technical feasibility of second-generation, investors not yet dare to invest on the new energy paradigm. Due to that reason, second-generation bioethanol ages under laboratory bench. The main reason that makes investor to hesitate in second-generation is the cost intensive pretreatment stage. Especially, the hindrance of pretreatment stage worsens when the production scale is increased. Around the world, researchers, investors, and government has been working to solve this scale up problem. Some of the approaches used to debottleneck the scale up problem of pretreatment stage were building demo company, pilot plant testing, advanced computer simulation and commercial biorefinery plant. Technically, the best way to test such problem is through demonstration and pilot plant testing. However, those approaches are cost intensive. For that reason, this research has proposed to investigate the scale up problems through advanced computer simulation. The cost of this method for testing the technical, technological, and economic feasibility of the sugarcane based biorefinery by building the superstructure plant in simulator is almost zero. In the simulator, production process, techno-economic analysis, environmental safety, and energy analysis will be performed safely and cheaply. Therefore, with some trade-off between reality and cost, the scale-up, which hinders investors not to invest on second-generation bioethanol production will be cleared through whole biorefinery plant process simulation and techno-economic analysis.

1.8 OBJECTIVE

1.8.1 General Objective

The main objective of this research was to investigate the problems of sugarcane bagasse-based bioethanol producing biorefinery plant and techno-economically analyze through advanced process simulation.

1.8.1.1 Specific Objectives

1. To collect relevant secondary data and information for the biorefinery plant modelling and simulation
2. To scale up and simulate the pretreatment, saccharification, cofermentation and distillation of bioethanol production from sugarcane bagasse
3. To analyze the feasibility of the sugarcane bagasse-based bioethanol producing biorefinery plant techno-economically

1.9 SIGNIFICANCE OF THE RESEARCH

The main goal of this research was to investigate the cellulosic ethanol technical and economic barriers and open the new door of liquid bioethanol production from sugarcane bagasse. So, the immediate significances of this research are scientific community, policy makers, and investors. The result of this research will also clear the fog that hinders investors not to invest their money on second-generation biofuel producing biorefinery plants. Beyond that, this research helps to march academicians to keep researching possibility of producing biofuel from sugarcane bagasse. In general, this research has value to academic researchers: It can also serve as a platform to give basic information on the bioethanol development to create further research on areas of data deficiency. The indication of areas lacking enough data and potential areas for additional study would direct researchers to select priority areas and undertake further study. Beyond business society, supply chain actors, policy makers, the socio-economic, techno-economic, and environmental benefits from this research.

CHAPTER 2: **LITERATURE REVIEW**

2.1 LIGNOCELLULOSIC BIOMASS

The sun is the ultimate source of energy for planet earth. Plants are the primary natural solar panels that directly capture the solar energy in the form of chemical bond. And they are considered as primary energy producers in the energy flow. The chemical bond created by photosynthesis ($6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$) is the biomass and the biomass become the blood and bone of another living things. As the above chemical reaction shows, photosynthesis is natural and eco-friendly. It only needs the CO_2 that we call air pollutant and produce the energy that we utterly depend on it. The chemical bond formed by the photosynthesis process matters whether a plant is woody or not. Thus, that have woody nature are sometimes called lignocellulosic plants. The main components of the lignocellulosic biomasses are cellulose, hemicellulose and lignin. Cellulose is a major structural component of cell walls, and it provides mechanical strength and chemical stability to plants. Hemicellulose is a copolymer of different xylose (C_5) and glucose (C_6 sugars that also exist in the plant cell wall. Lignin is polymer of aromatic compounds produced through a biosynthetic process and forms a protective layer for the plant walls.

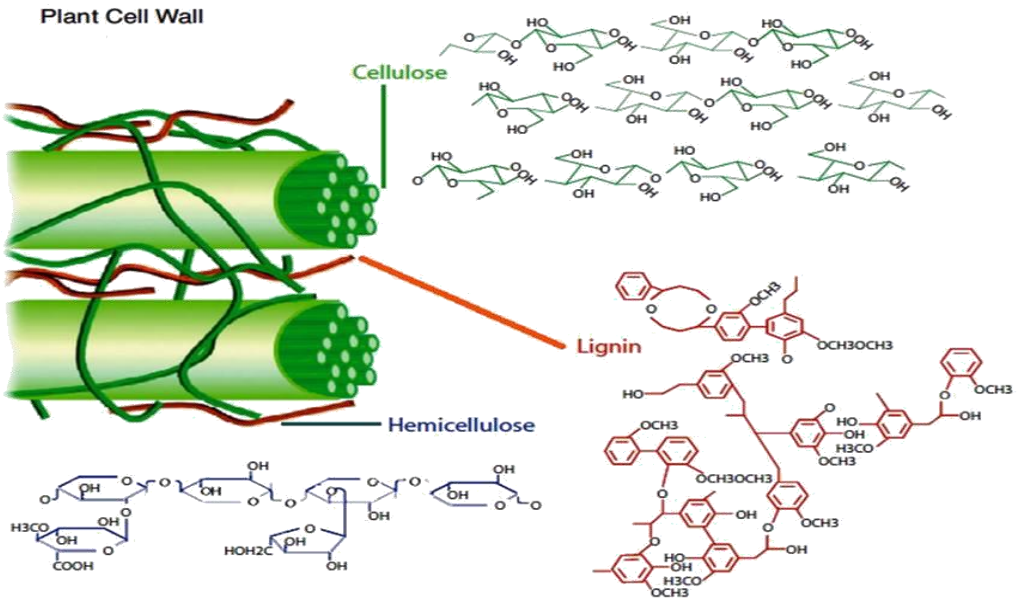


Figure 7Microscopic Structure of Lignocellulosic Biomass (Mussatto and Teixeira 2010)

In nature, biomass grows and as well decays during the year. It has been estimated that around $7.5x10^{10}$ tonnes of cellulose are consumed and regenerated every year(Michels,

Wagemann, and Main 2010) (C.L. Lkoli, 2014). It is thereby the most abundant organic compound in the known world. In addition to the three basic chemical components found as part of lignocellulose, water, protein, ash content and other extractives are available. The chemical composition of lignocellulose highly depends on its source. There is a significant variation of the lignin and hemicellulose content of lignocellulose depending on whether it is derived from hardwood, softwood, or grasses.

Table 3 Composition of lignocellulose in several sources on dry basis (Sun and Cheng 2002)

Lignocellulosic materials	**Cellulose (%)**	**Hemicellulose (%)**	**Lignin (%)**
Hardwoods stems	40–55	24–40	18–25
Softwood stems	45–50	25–35	25–35
Nut shells	25–30	25–30	30–40
Corn cobs	45	35	15
Grasses	25–40	35–50	10–30
Waste paper from offices use	85–99	0	0–15
Wheat straw	30	50	15
Sorted refuse	60	20	20
Leaves	15–20	80–85	0
Cotton seed hairs	80–95	5–20	0
Newspaper	40–55	25–40	18–30
Waste papers from chemical pulps	60–70	10–20	5–10
Primary wastewater solids	8–15	NA	24–29
Swine waste	6.0	28	NA
Solid cattle manure	1.6–4.7	1.4–3.3	2.7–5.7
Coastal Bermuda grass	25	35.7	6.4
Switch grass	45	31.4	12.0
Coffee husk	27.65	2.3	0
Eucalyptus tree	46.6-50.3	12.7-14.4	26.9-8.2
Sugarcane Bagasse	31.9-43.4	12.2-25.5	23.1-7.6

2.1.1 Cellulose

Cellulose is the β-1, 4-polyacetal of cellobiose (4-O-β-D-glucopyranosyl-D-glucose). Cellulose is more commonly considered as a polymer of glucose because cellobiose

consists of two molecules of glucose. The chemical formula of cellulose is $(C_6H_{10}O_5)_n$ and the structure of one chain of the polymer:

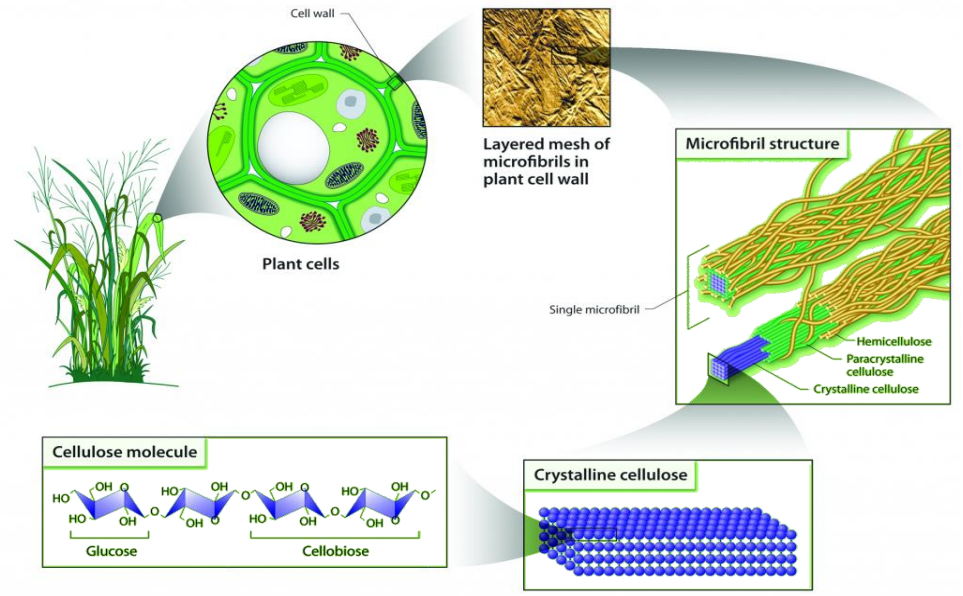


Figure 8 Cellulose molecule structure (Carvalheiro, Duarte, and Gírio 2008)

Many properties of cellulose depend on its degree of polymerization (DP), i.e. the number of glucose units that make up one polymer molecule. The DP of cellulose can extend to a value of 17000, even though more commonly a number of 800-10000 units is encountered (Kirk and Farrell 1987). For instance, cellulose from wood pulp has a DP between 300 and 1700. The nature of bond between the glucose molecules (β-1,4 glucosidic) allows the polymer to be arranged in long straight chains. Hydroxides are evenly distributed on both sides of the monomers, which allow it for the formation of hydrogen bonds between the molecules of cellulose. The hydrogen bonds in turn result in the formation of a compound that is comprised of several parallel chains attached to each other (Faulon *et al.*, 1994). Cellulose is found in both crystalline and amorphous structure. The coalescence of several polymer chains leads to the formation of microfibrils, which in turn are united to form fibrils. In this way cellulose can obtain a crystalline structure.

2.1.2 Hemicellulose

The term hemicellulose is a collective term. It is used to represent a family of polysaccharides such as arabino-xylans, gluco-mannans, galactans, and others that are found in the plant cell wall and have different composition and structure depending on their source and the extraction method. The most common type of polymers that belongs

to the hemicellulose family of polysaccharides is xylan. The molecule of a xylan involves 1->4 linkages of xylopyranosyl units with α-(4-O)-methyl-D-glucuronopyranosyl units attached to anhydroxylose units. The result is a branched polymer chain that is mainly composed of five carbon sugar monomers, xylose, and to a lesser extent six carbon sugar monomers such as glucose. Important aspects of the structure and composition of hemicellulose are the lack of crystalline structure, mainly due to the highly branched structure, and the presence of acetyl groups connected to the polymer chain (Zhuang, 2007). Hemicellulose extracted from plants possesses a high degree of polydispersity, polydiversity and polymolecularity. However, the degree of polymerization does not exceed the 200 units whereas minimum limit can be around 150 monomers. Hemicellulose is insoluble in water at low temperature. However, its hydrolysis starts at a temperature lower than that of cellulose, which renders it soluble at elevated temperatures (Humbird, 2011). The presence of acid highly improves the solubility of hemicellulose in water.

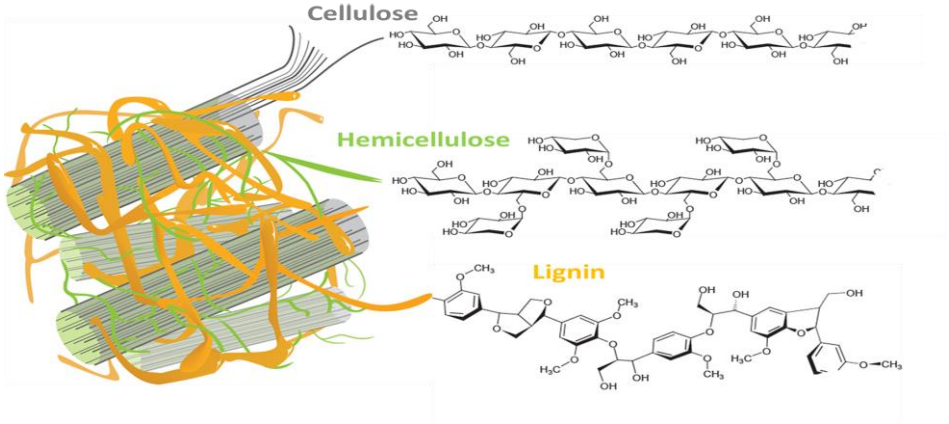


Figure 9 Schematic representation of hemicellulose backbone of arborescent plants

2.1.3 Lignin

Lignin is the most complex natural polymer. It is an amorphous three-dimensional polymer with phenylpropane units as the predominant building blocks. More specifically, p-coumaryl alcohol, coniferyl alcohol and sinapyl alcohol are the ones most commonly encountered. Dividing higher plants into two categories, hardwood (angiosperm) and softwood (gymnosperm), it has been identified that lignin from softwood is made up of more than 90% of coniferyl alcohol with the remaining being mainly p-coumaryl alcohol units. Contrary to softwoods, lignin contained in hardwood is made up of varying ratios of coniferyl and sinapyl alcohol type of units(Cragg et al. 2015).

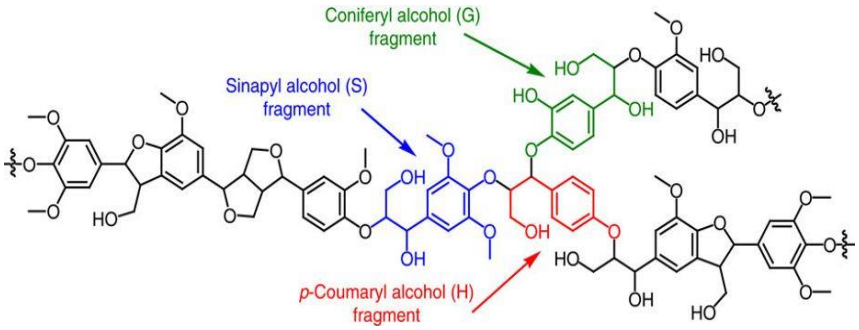


Figure 10 Components of lignin structure

2.1.4 Extractives and Ash

Extractives and ash are also components in biomass, but are usually very low, below 5 % and around 1 % respectively. The three main groups of softwood extractives are terpenes, fats, and waxes but there are also other compounds present such as n-alkanes. The inorganic compounds that remain after burning the organic matter is called ash.

2.2 SUGARCANE BAGASSE PRETREATMENT TECHNIQUES

Sugarcane bagasse is the feedstock used for the bioethanol production. Although lignocellulosic biomass is the most abundant source of bioethanol, it has not been widely used to produce biofuel. The immediate use of bagasse as energy source is in the form of fire wood. This is because the biomass has interlinked bond of component. Due to that interlinked chemical bond, the hydrolysis process in the biorefinery process becomes so slow and rate-limiting step. The hydrolysis step is the main factor to incorporate the most cost intensive pretreatment step. Pretreatment is the process of altering the internal structure of the lignocellulosic biomass and it makes it accessible for enzymatic hydrolysis. Due to this energy intensive step, investors hesitate to invest their money in the biorefinery business area. Researchers have been investigating the optimization of this step.

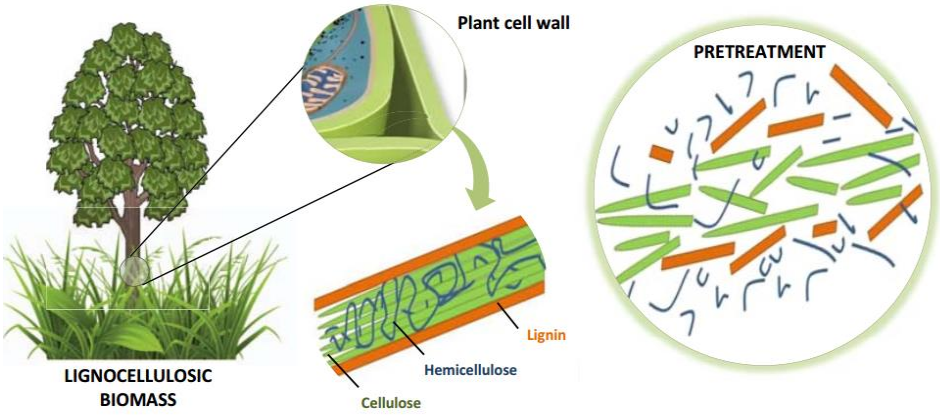


Figure 11 Effects of pretreatment on lignocellulosic biomass (Hsu et al, 1980)

Possible goals of pretreatment include the removal of lignin and disruption of the crystalline structure of cellulose. Effective and economical pretreatment techniques meets to (1) deconstructing the three-dimensional structure of bagasse, modifying its polymerization degree and decreasing the cellulose crystallinity; (2) increasing the surface area and porosity of the bagasse; (3) generating highly digestible pretreated solids and promoting high sugar yields after hydrolysis (cellulose conversion yields greater than 90%); (4) avoiding the formation of fermentation inhibitor compounds (especially acetic acid from hemicellulose, furfural and hydroxymethylfurfural from sugar degradation, and phenolic compounds from lignin degradation); (5) allowing hemicellulose and lignin recovery for subsequent use on the production of valuable coproducts; (6) requiring a low demand of post-pretreatment operations such as washing and neutralization; and (7) requiring minimal energy, chemicals, and water inputs and using simple, reasonably sized, and low-cost reactors. Ideally, the pretreatment employed leads to a limited formation of degradation products that inhibit enzymatic hydrolysis and fermentation, and is cost effective. Nevertheless, those are the most important challenges of current pretreatment technologies. There are many different techniques of pretreatments. Those pretreatments vary based on different factors like technical, economic, environmental and others. The most common methods of pretreatment techniques are listed below. Choice of pretreatment technique depends on the type of final product that the company going to produce. Therefore, different biorefinery companies can follow different routes of pretreatment. Depending on different factors, the pretreatment techniques chosen for this biorefinery plant is diluted sulfuric acid followed by enzymatic hydrolysis.

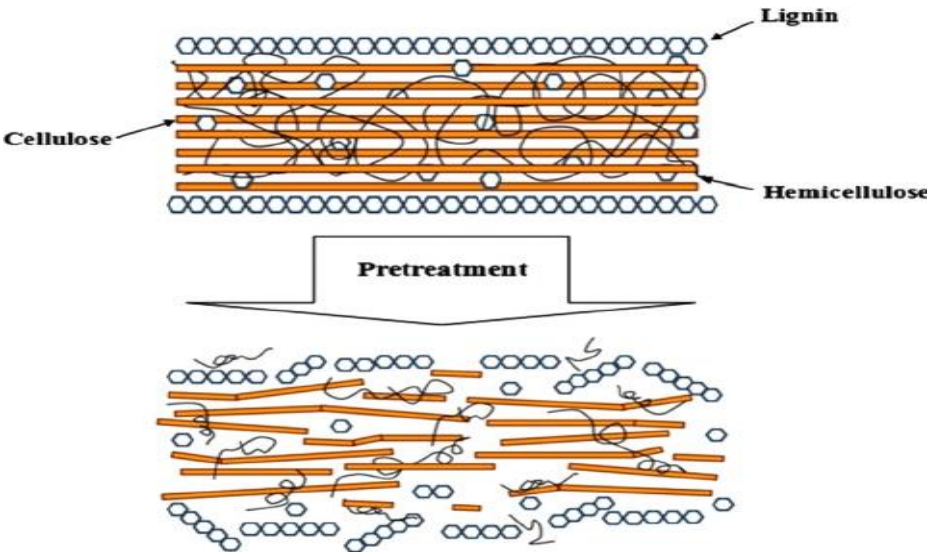


Figure 12 Feedstock after and before pretreatment

2.2.1 Physical Feedstock Handling

Physical pretreatment or feedstock handling involves mechanical processing such as chipping, grinding, and milling, to reduce both particle/chip size of the raw material, and the crystallinity of cellulose. If this is done to a high extent, it is often seen as a separate form of treatment. However, it is often used in combination with other forms of treatment, to help speed up the process. Steam explosion is often considered a physical treatment, as it does not involve any use of chemicals, except water(Modenbach and Nokes 2013). The raw material is exposed to steam at high pressure and temperature, degrading both hemicellulose and lignin. The pressure is then rapidly decreased, causing high mechanical stress on the material, causing it to break apart. The process can also include the use of acids and alkali, to increase the degradation of lignin and hemicellulose.

2.2.2 Chemical Pretreatment

Chemical pretreatment often involves the use of reactive chemicals at elevated temperature and pressure. A range of chemicals has been used for feedstock pretreatment purpose. Some of the chemicals used by different researchers are acids, alkali, ozone, strong oxidizers, organic solvents, or even specific microorganisms. The mechanisms and rates at which the chemicals alter the feedstock structure varies. Lignin and hemicellulose are degraded, while crystalline cellulose is transformed into an amorphous state(Kamm 2014). After pretreatment, the raw material structure is more susceptible for further saccharification of cellulose. Acid hydrolysis, the use of mineral acids such as hydrochloric acid, phosphoric acid and sulfuric acid is one of the most commonly used methods of hydrolyzing lignocellulosic materials. The 2012 bioenergy report of NREL has used sulfuric acid for pretreatment and as a regular hydrolyzing agent(Schwab et al. 2016). This is done by using concentrated sulfuric acid at relatively low temperature (50-150 °C), or by using dilute acid at elevated temperature (150-300 °C)(Sindhu, Binod, and Pandey 2016). Using concentrated acid as a method for pretreatment or hydrolysis cause several difficulties that must be overcome, such as toxicity, corrosion, and acid recovery. Dilute sulfuric acid however is easier to handle, and is the preferred choice in industry. Hemicelluloses are easily hydrolyzed in dilute acid, while cellulose are more resistant. Achieving high yields of glucose also has the effect of degrading hemicellulose monosaccharides into degradation products, such as furfural and 5-Hydroxymethylfurfural (5-HMF). Such compounds are known to have significant inhibitory effects on the fermentation of sugar. An often-preferred solution is to use a combination of acid hydrolysis and enzymatic hydrolysis in two stages. The acid

hydrolyses the hemicellulose fraction, while at the same time serving as a form of pretreatment for the cellulose fraction. The hemicellulose fraction is solubilized and the cellulose is altered into a more amorphous state, which makes enzymatic hydrolysis in the next stage possible (Humbird, 2011). Cellulose is hydrolyzed into glucose, which can further degrade into 5-HMF, which decomposed into levulinic and formic acid.

2.2.3 Enzymatic Hydrolysis of Cellulose

As mentioned earlier, a solution could be to hydrolyze the cellulose fraction of lignocellulose by enzymes. Cellulose is hydrolyzed to glucose by the enzyme complex called *cellulase*, which is produced by *Trichoderma reesei,* a filamentous fungus capable of degrading cellulose(Dashtban, Schraft, and Qin 2009). The enzyme complex consists of three components. Endo-*β*-(1, 4)-glucanase (Cx-cellulase) breaks random bonds in amorphous regions of cellulose molecules, while exo-*β*-(1,4)-glucanase (cellobiohydrolase) removes cellobiose unites from the non-reducing ends of cellulose molecules. To get a complete conversion of cellulose into glucose, a *cellobiose* [*β*-(1,4)-glucosidase] must be present(Dashtban et al. 2009). Industrial cellulases normally contain enough levels of cellobiose. Enzymatic hydrolysis of hemicelluloses is also possible, but is more complex. Complete utilization of hemicellulose requires a blend of several different hydrolytic enzymes. Commercial cellulases often contain hemicellulase activities, especially for the use on corn stover, where yield approaching 80% are achieved(Subhedar and Gogate 2013). However, the preferred industrial solution for most lignocellulosic material is to use dilute acid for hemicellulose hydrolysis, and cellulase enzyme.

2.2.4 Fermentation

Hydrolysis of lignocellulosic material yields a mixture of sugars including glucose, xylose, mannose, arabinose, and galactose. Currently, many different strains of microorganism are identified that able to ferment glucose in industrial scale (e.g. *Saccharomyces Cerevisiae)*. However, a strain that able to ferment both glucose and xylose at the same time is limited. The most known strain that able to co-ferment both glucose and xylose is Z. Mobilis (Zhao et al. 2012). Therefore, condition will set to develop microorganisms capable of metabolizing other sugars in a mixture with glucose. Moreover, parameters, which can affect fermentation, will set on optimum conditions. Some of the most common and adjustable parameters to be set on their optimum condition are temperature, pH, feedstock, and product concentration. The co-fermentation process produces a fermentation broth called ‘beer’.

2.2.5 Bioethanol and other Solid Material Recovery

When ethanol is produced from renewable biomass through biochemical process, it is called bioethanol. Bioethanol utilization as biofuel has the advantages of being both a renewable and an environmentally friendly fuel source. Alternative technology options are suggested for bioethanol recovery such as distillation, and pervaporation. Difference in the volatilities of substances in the fermentation broth is the prerequisite for separation by distillation columns. The volatile compound evaporates and the vapor moves upward and leaves the column at the top. The high-boiling compounds, which remained in the liquid phase move downward, and leave the column at the bottom. In bioprocesses, it is employed for the recovery of large-volume, low-boiling products such as ethanol. Membrane systems, such as pervaporation, have become viable alternative to traditional separation methods such as distillation columns which are energy intensive (Hamelinck, Hooijdonk, and Faaij 2005). In pervaporation, membranes are utilized with liquid feed on one side, and a low-pressure permeated gas on the other side. Due to lower required heat input in pervaporation, this process can save on cost associated with the heat and steam needed for the reboiler of distillation columns. However, membrane cost and life expectancy of the membrane are two important factors, which should be considered to compare the efficiency of this separation technology with distillation column.

The immediate product of fermentation is a mixture of desired product, undesired products, cell mass and water which needs to be purified. The technologies for purification depend on the type of products recovered. All the technologies in downstream processing use one or several differences in the chemical and physical properties of the desired product from other materials. For instance, in cases where fermentation products are more volatile than water, recovery by distillation is the technology. More than 90% of the fermentation broth is also water(Aden et al. 2002). So, the best technology to separate ethanol from water is distillation. Separation beyond distillation is performed by vapor-phase molecular sieve adsorption and other upgrading to fuel level techniques.

CHAPTER 3: **DESIGN & SIMULATION BASIS**

Process simulation stands for the model- based depiction and design of chemical, physical, biological, and other technical processes unit operations by executing the appropriate mass and energy balances. Basic preconditions are an in-depth familiarity with the chemical and physical properties of pure components and mixtures, of reaction kinetics and mechanisms, and of mathematical modeling techniques, which, jointly, enable the software-based design of a process.

Process simulation history is intimately connected with the progression of computer science and hardware as well as the development of programming languages. It was not until the 1970s that proper software and hardware became available and the first applications of chemical process simulation were implemented. However, the modeling of chemical properties was possible long before the existence of such software. The cubic equations of state and the Antoine equation, for example, were available during the previous century. The main interface for modern process simulation software is, generally, a representative flow diagram where the user is prompted to position and connect with streams (energy or material) the various unit operations. The software solves mass and energy balance equations, usually in their steady state form, to compute a stationary operating point. At all times, process simulations utilize models that are associated with approximations and assumptions but gives the opportunity to the user to describe a property within a broad range of conditions (such as temperature and pressure), which are not necessarily found in the literature.

Process simulation is frequently carried out during the design phase or in advance of the full operation of a plant to test how changes in unit operation specifications can affect a procedure throughout the duration of its life cycle. By utilizing process simulation software, the user can set up and compare alternative but equivalent process routes and thereby select the preferred option based on cost, energy consumption, carbon footprint, or other criteria.

There are several simulation packages used by process industries for simulating, analyzing, and optimizing their various processes, to achieve efficient operations and maximize their profits. Simulation packages are used for generating high-accuracy predictive information, which will aid decision making and supports decisions regarding the product and process innovation, design, and operation. Among these packages are Aspen Plus (by AspenTech), Aspen Hysys (by AspenTech), Pro/II (by SimSci), ProSimPlus (by ProSim), SuperPro (by Intelligent, Inc.), Unisim (Honeywell), ChemCAD (from Chemstations, Inc.), gPROMS

(from Process Systems Enterprise Limited [PSE]), and so on, have been successfully used by process engineers and scientists in simulating and optimizing complex conventional processes. Some of these simulators were designed specifically for a type of reaction, for example, simulators designed specifically for bioprocesses that include Bioprocess Simulator (by AspenTech), Biotechnology Design Simulator (BDS developed by Life Sciences International Philadelphia, PA), SuperPro Designer (developed by Intelligent, Inc.), and BATCHES (from Batch Process Technologies) have been found; all designed for bioprocesses.

3.1 DESIGN BASIS

3.1.1 Plant Capacity and Attainment Estimation

Products of biorefinery are more expensive than similar products of petroleum refinery. This is because biorefinery trades-off some economic advantages for the sake of the environment and society health protection. Bioethanol decreases with increasing the biorefinery plant production capacity. When the source of feedstock is from farm land, there is a need of lands to operate the plant in full capacity. The raw material for this biorefinery plant is sugarcane bagasse. The source of the bagasse is mainly from sugar factories. The sugar factories may be more than one. Therefore, to increase the production capacity, the land for crop production or number of factories for bagasse collection increases. This additional radius added to increase crop production have marginal cost(Nguyen and Prince 2006). To overcome the dilemma of cost and capacity, designing the optimum plant capacity is important. This process of redesigning the optimum plant capacity helps for market penetration. Biorefinery plant optimum capacity estimation modeling discusses the mathematical modeling by referring literatures, observations, and other surveys. This model also discusses the trade-off between energy, environment, and economy. Increasing the plant capacity, increases the cost of feedstock. So, by taking a tonne of bagasse feedstock as a sample from field or sugar factory to plant gate, the optimum plant capacity can be estimated using Nguyen and Prince method(Nguyen and Prince 2006):

Distance changes from x to (x + dx). [1]

Quantity of crop grows $dM = 2\pi \mathrm{Y}a$ [2]

Cost of transportation $dc = \pi x\ dx Y a k b\ x$ [3]

Where; α= fraction of useful land, γ = Agricultural yield per unit area, k = transport cost per unit distance and unit mass and β = ratio of actual road length to direct distance. Based on the above premises, the total cost of all crops up to the distance of x is

$$C = \int_0^x 2\pi Yakbx^2\, dx \;=\; \frac{2}{3}\pi\, Yakbx^3 \qquad [4]$$

and the total transported quantity of crop becomes [5]

$$M = \int_0^x 2\pi aYx\, dx \;=\; \pi Yax^2 \qquad [6]$$

Then, $P = \frac{M}{y}$ [7]

Where; y is the annual fractional product. Hence, the required x for the above plant capacity, P is [8]

$$X = \left(\frac{P}{\pi YAy}\right)^{0.5} \qquad [9]$$

According to Overend (2006), the transport cost then varies with capacity to the power of 1.5(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006)(Nguyen and Prince 2006). Then, the total cost (TC) of a factory operation may be represented as

$$TC = A.P^m + B.P^n + k'.P$$

Where; A = transport cost factor, m = capacity exponent for transport, found as 1.5, B = production costs factor, n = capacity exponent for production costs (generally around 0.7) and k' = overhead costs, which is constant per unit of product. Hence C, cost per unit quantity of product ($/t) can be expressed as:

Equation 1 Plant Capacity Estimation Model

$$C = \frac{TC}{P} = A.P^M + B.P^{-N} + k' \qquad [10]$$

Where: M = m-l, N = 1 - n; At optimum (least cost) plant capacity P [11]

$\frac{dC}{dP} = 0$ hence, $\frac{dC}{dP} = MAP^{(M-1)} - NBP^{(-N-1)} = 0$ [12]

$$MAP^{(M+N)} = NB \quad [13]$$

$$P^{(M+N)} = \frac{NB}{MA} \quad [14]$$

Let us denote the ration of transport to production cost as R: then [15]

$$R = \frac{AP^{M}}{BP^{-N}} = \frac{A}{B}(P)^{(M+N)} \quad [16]$$

Hence at the optimum, $R = \left(\frac{A}{B}\right)\left(\frac{NB}{MA}\right) = \frac{N}{M}$ [17]

Based on the plant capacity model, the minimum total cost of the plant should be N/M, which is a quantity not dependent directly on the actual costs, but only on the scale factors of the transport and production costs. So that, n usually varies between 0.6 and 0.8, N lies between 0.4 and 0.2(Nguyen and Prince 2006). the researcher, M. H. Nguyen et.al. had derived m as 1.5. Hence M would be between 0.5 and 1. The ratio of the two-unit costs of transport and production would then lie at the optimum in the range of 0.2 to 0.8, with values around 0.4 to 0.6 as most likely(Nguyen and Prince 2006). Using the above model, the size of this biorefinery plant is estimated to be 2,000 metric tonne of bagasse per day. This is the optimal capacity for market penetration with expected minimum ethanol selling price (MESP)(Rodrigues Gurgel da Silva, Errico, and Rong 2018).

After estimating the plant capacity, the plant attainment is also estimated to be 95.94%. The percent of attainment number comes from the above plant capacity estimation model and survey of different related papers. Most of the literature recommends the plant attainment of chemical industry to be in between 90-95%(Xu, Singh, and Himmel 2009). This biorefinery plant is expected to work about 8,410 hours a year by considering holidays, maintenance, and other related conditions. Then, the percentage of this biorefinery plant attainment is estimated as

$$Plant\ Attainment = \frac{Working\ hours}{Total\ hours} * 100 = \frac{8410}{8766} * 100 = 95.84\%$$

With the above percentage of plant attainment, the daily required sugarcane bagasse feedstock is 2,000 metric tonnes. Then, using the 96% plant attainment, the annual feedstock requirement is about 700,000 dry tonnes. This much amount of blended feedstock is expected to be purchased from industrial by-products (bagasse, paper, and coffee husks), agricultural wastes and collect from municipal wastes and self-grown green lignocellulose biomasses.

3.1.2 Production Process Modes

The overall operation mode of the biorefinery plant will be continuous mode. However, some equipment or modules of the plant like seed fermenters, enzyme production and product purification will work batch-wise. In addition to that, the bioprocess will be considered as steady process. Although there is temporal variation during operation, overall process is considered as steady state process by neglecting some insignificant time variabilities.

The two most important production process steps are saccharification and fermentation. So, the mode of the two enzymatic reaction are also specified. The intermediate product from pretreatment is cellulose. This cellulose must change through saccharification into glucose (C_6) and xylose (C_5). The process of converting cellulose into glucose and xylose needs an enzyme called cellulase. The fungus used to produce cellulase is Trichoderma Reesei(Xu et al. 2009). After converting cellulose into hexane (glucose) and pentane (xylose) sugar, co-fermentation will follow. When the saccharification is followed by co-fermentation, it is called sequential mode. The group of bacteria that convert glucose and xylose into ethanol are called Zymomonas Mobilis(Gao et al. 2012). The fermentation design is co-fermentation, means Zymomonas Mobilis bacterial strain converts both hexose and pentose sugars at the same time and in the same fermenter. Therefore, the overall enzymatic reaction is in sequential simultaneous co-fermentation mode (SSCF).

3.2 SIMULATION ENVIRONMENT BASIS

3.2.1 Aspen Plus Version 11 Setup

Aspen plus is advanced simulation software. The program was originally developed by the Massachusetts Institute of Technology for the U.S. Department of Energy to evaluate synthetic fuel technologies. The program includes a library of standard unit operation blocks (e.g. mixers, pumps, heat exchangers, reactors, splitters, columns, and so on), which represent processes taking place in an actual chemical plant. The simulation of a process plant is done by specifying configurations of unit operations and the flow of material, heat, and work streams. Aspen Plus also has an extensive components database containing physical properties of many pure components. Within the program there exist mathematical routines (convergence algorithms) for solving different equations of material and energy balances as well as equilibrium equations. Aspen Plus uses a sequential-modular approach to flow sheet convergence, where mass and energy balances for individual unit operation

blocks are computed sequentially. Property, Simulation, Safety analysis and Energy analysis are four of the main categories.

Besides the unit operation blocks, Aspen Plus utilizes other mechanisms to access variables in simulating chemical processes. Those model performance analysis techniques include Fortran blocks (calculator), sensitivity analysis, optimization, and design specifications. Fortran blocks are used for feed-forward control and allow incorporation of user code into a model to control variables in an Aspen Plus flow sheet. Design specification is used for feedback control, allowing the user to set design values for any flow sheet variable or function of flow sheet variable. The design specification varies the manipulating flow sheet variable, feed stream or block input, to achieve the design value. To compute design specification function values, Fortran statements can be used within the design specification block. Aspen Plus is also able to handle recycle streams, using a feature called “tear-streams”. Stream and block variables must be manipulated iteratively, to converge upon the mass and energy balance, until it obtains a solution. To be able to construct a process model in Aspen Plus, the following six steps are very recommendable({Aspen Technology 2000).

I. Setup the aspen plus global environments
II. Specify all the reactant, intermediate and product components
III. Align all the unit operations in logical, sequential, and modular manner
IV. Specify all the necessary operating conditions like temperature, pressure, concentration, heat duties etc., for each unit operation, inlet, and/or outlet streams.
V. Run the simulation and get the result summary
VI. Analyze the results against safety, energy, economic and other perspectives.

3.2.2 Selection of Property Package

Aspen Plus V11 is rich in thermodynamic property packages. The property method is chosen based on the nature of the interaction of the components in the process. The process of selecting the suitable model is more of the process of comparing the obtained predictions with data from the literatures. If the components in one specific reaction behaves ideality, one property package from equation of state is selected. If the available component interacts, the property package will be selected from activity coefficient model. The interaction among components comes from polarity, irregular shape, and not-uniform size of feedstock components. The Equation of State (EoS) models are used for predicting properties for most hydrocarbons and other non-polar components. The type of physical property packages available

in Aspen Plus v11 software. Some of the most popular property method in Aspen Plus for such type of process simulation includes, the Peng-Robinson equation and the Soave-Redlich-Kwong equation, and variations of these. Activity model handles highly non-ideal systems and by nature are more empirical than EoS models. These models are mostly used for non-ideal systems or polar components. It is common to use an EoS model to predict vapor behavior, and use an activity model for the liquid phase. Since activity models are empirical, the application is limited to the data range used to predict its parameters. The property package selection assistant uses the following process to specify the best package for any process.

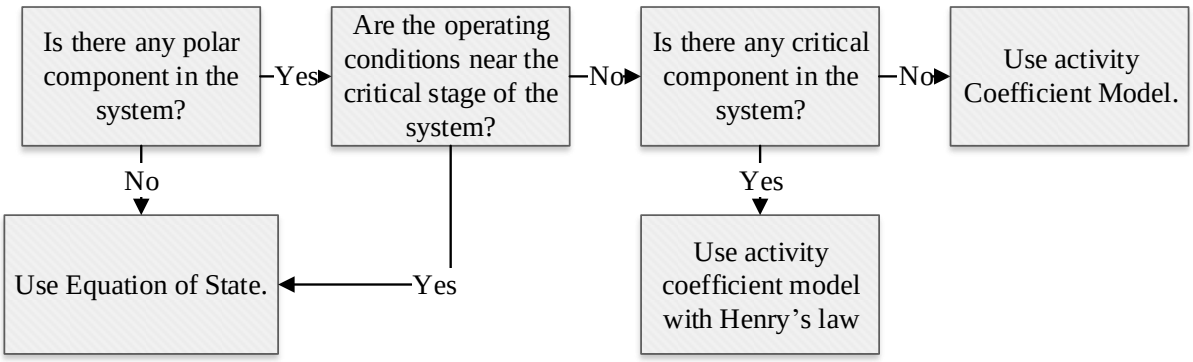


Figure 13 Property Package selection method flowsheet diagram

Vapor Pressure models are used at low pressures for ideal mixtures, such as hydrocarbon systems and mixtures of slightly polar ketones and alcohols. This system consisting of mainly water and ethanol and is considered non-ideal. Mixtures of water-ethanol forms azeotropes(Strømsnes 2016). The Non-Random-Two-Liquid (NRTL) equation and the Universal Quasi Chemical (UNIQUAC) equation have been used to successfully represent such systems. Both property models use a combination of temperature and non-temperature dependent parameters to calculate each components activity coefficient. They are good choices for representing both vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE), although UNIQUAC is more detailed, and applicable for a broader range of components, NRTL thermodynamic property method is chosen for this biorefinery plant.

Equation 2 NRTL property package final equation

$$ln\,\gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \left(\frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \right) \quad [18]$$

$$G_{ij} = exp(-\alpha_{ij}\tau_{ij}) \quad , \quad G_{ii} = 1 \quad [19]$$

$$\tau_{ij} = a_{ij} + b_{ij}/T + e_{ij}\,ln\,T + f_{ij}T\,, \tau_{ii} = 0 \quad [20]$$

$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15) \quad [21]$$

Where; The binary parameters a_{ij}, b_{ij}, c_{ij}, d_{ij}, e_{ij} and f_{ij} can be determined from VLE and/or LLE data regression. The Aspen Physical Property System has a large number of built-in binary parameters for the NRTL model(Neubauer and Pesaran 2013).

3.2.3 Estimating Binary Coefficient

Binary coefficients are important for accurate representation of equilibria for both pure components and mixtures. In this work, vapor-liquid equilibria (VLE) of binary mixtures containing water and ethanol is important. Binary coefficients for these components are provided natively binary coefficients can either be obtained directly from the literature, or experimental data of equilibrium behavior can be used to calculate the coefficients by regression. Aspen plus provides an automated function for parameter estimation based on the UNIFAC (UNIQUAC Functional-group Activity Coefficients) group-contributing method. It predicts interactions between molecules by applying standardized contributions for functional groups present on the molecules that make up the liquid. The components of special interest in this work, such as water, ethanol and acetic acid have well defined values for this method. Binary coefficients used in this work are all estimated by using the UNIFAC estimation method with emphasis on representing vapor-liquid equilibria. One drawback of using only one property package based on activity coefficients is that simultaneous representation of VLE and LLE behavior is difficult. The obtained binary coefficients are almost always a compromise between the two. Some properties of the most important mixtures are given in the following figures. All the plots are at atmospheric, as most of the processes are performed at or slightly above 1.0 atm.

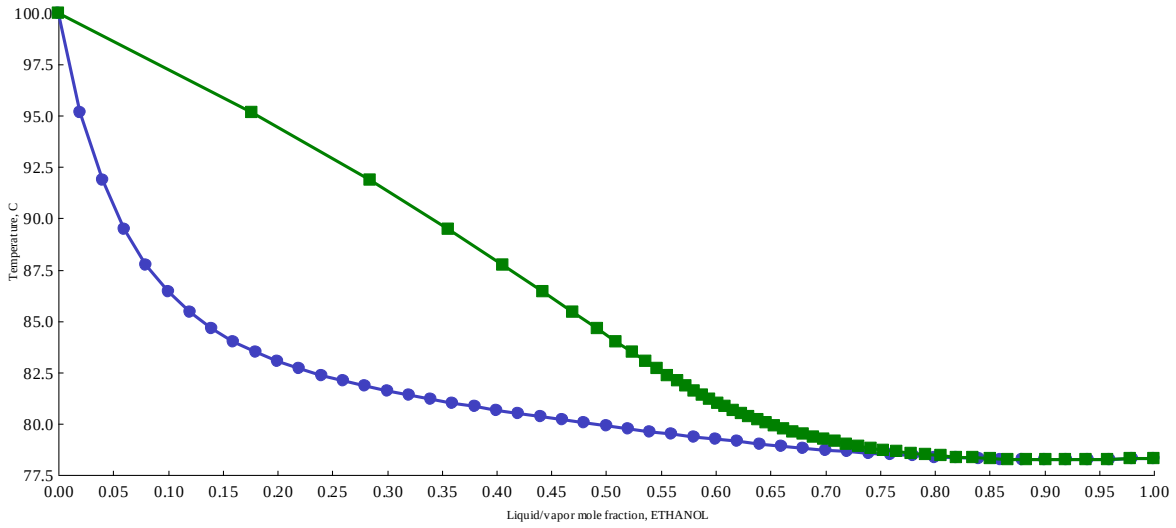


Figure 14 A T-xy diagram that shows the azeotropic point of ethanol and water

The above figure is directly plotted by Aspen Plus v 11 by varying ethanol. It shows, the equilibrium composition of ethanol and water using T-xy diagram. As the graph indicates, the azeotropic point is at about 78 wt%. This match with experimental result referred from different literature.

3.2.4 Input Component List

The feedstock used for this biorefinery plant is sugarcane bagasse. It has different components. The physical and chemical composition of sugarcane bagasse is analyzed proximately and ultimately. The list of components and their composition in sugarcane bagasse is taken from NREL design report and other related research institutes. The list of components used in this biorefinery plant simulation are attached in appendix-1. The component list contains pure, mixture, solid, liquid, and gaseous phases. One of the main reasons for selecting Aspen Plus for this plant simulation was that, Aspen plus can handle all the phases and its huge property package databases for almost all components. Although Aspen Plus contain huge database of components, some of the components of the feedstock are not available in its library. However, Aspen Plus has also user-friendly interface. Some of the non-library components are can inserted by referring their thermodynamic property in different literatures.

Some of the non-library components, which are inserted for this model includes all pentosans, which are modeled as xylan and all hexosans are modeled as cellulose. Cellulose is modeled as a crystalline component (Cellulose C) and an amorphous component (Cellulose A). Cellulose A is a duplicate of Cellulose C, and meant to represent the amorphous cellulose and the hexosan fraction of hemicellulose. In general, those components can categorize into solid, liquid, and gaseous states. So, the reaction, the treatment and other performances consider all those component states.

CHAPTER 4: **METHODOLOGY**

4.1 DATA COLLECTION

The biorefinery plant is conceptually designed and simulated in Aspen Plus simulation software version 11. Most of the data used in this plant simulation was specified from the software's databank and others from international research centers around this field. Some design specific data were needed for the simulation process. Those data were collected from different authorized sources. The conceptual process modeling encompasses about 9 modules. Each and individual modules need specific type of data to run in the simulation software environment. For that reason, the design specific data were collected from different sources. Although most of the data were collected from secondary sources, they all were from authorized bodies or documents. Those sources of data were mainly from published literatures, reports, seminars, books, software databanks, supplier brushers and others.

4.1.1 Data for Upstream Processing

The data for upstream processing were the data used to make things ready for fermentation process. Most of the data collected for the upstream process were for the module of feedstock handling and pretreatment. The specific usage of the collected data in the feedstock handling module was used for feedstock selection, composition of feedstock, feedstock cost estimation, amount of feedstock needed to fully operate the plant and others. Those different types of data were collected from different authorized sources. Most of the data were collected from NREL design report, Idaho national laboratory and Harries group. Beyond those main sources other local and global sources were used. The labor cost for feedstock collection, transportation and other cost were determined based on the local market. Pretreatment module was also needing a lot of input data. Some of the most common input data for pretreatment module includes concentration and amount of sulfuric acid, pretreatment condition information and ammonia conditioning. That information also collected from different sources. In addition to the collected input data survey and observation methods were used.

Enzymatic hydrolysis and co-fermentation module need specific type of input data. For this module different sources were used. The most common and authorized sources for this module were NREL design report 2012. The type of data used in this module includes type of microorganisms, reaction conditions, fermentation periods, type of intermediate products,

rate of reaction conversions, amount of solid and liquid contents and others. Those all information was collected and inserted into the Aspen Plus library. After the co-fermentation and enzymatic hydrolysis bioprocess run for some duration of times, huge amount of data has generated.

4.1.2 Data for Downstream Processing

Downstream process needs massive amount of data. The most important module in the downstream process is product recovery. However, other modules can also be considered to fully simulate and analyze the biorefinery plant. All those downstream process sections need input data and information to perform meaningful work. Especially the product recovery module, distillation. The number of stages, running conditions, percentage of separation and other related data were need some authorized experimental resources. The resource for the downstream process were different for the different parts. In addition to the above raw experimental data, other information about the simulation software itself and the techno-economic analysis were also collected from other financial sources. The data collected in here were used to decide the interest rate, discount cash flow, internal rate of return, payback period, the plant life, depression cost, contingency rate, equity financing, cost indexing, supplier quote and other related data. Those all information had been collecting from different authorized sources before the simulation process has started. The result of the simulation using the above collected data were also analyzed in terms of environmental and energy integration.

4.2 CONCEPTUAL PROCESS MODELING

The paper uses a biochemical conversion pathway by referring a model developed by NREL. It also uses co-current dilute-acid pretreatment of blended feedstock handling, and enzymatic hydrolysis of the remaining cellulose, followed by co-fermentation of the resulting glucose and xylose to produce ethanol. The process design also incorporates onsite enzyme production, purchased and product storage, product purification, wastewater treatment, energy recovery, and utilities.

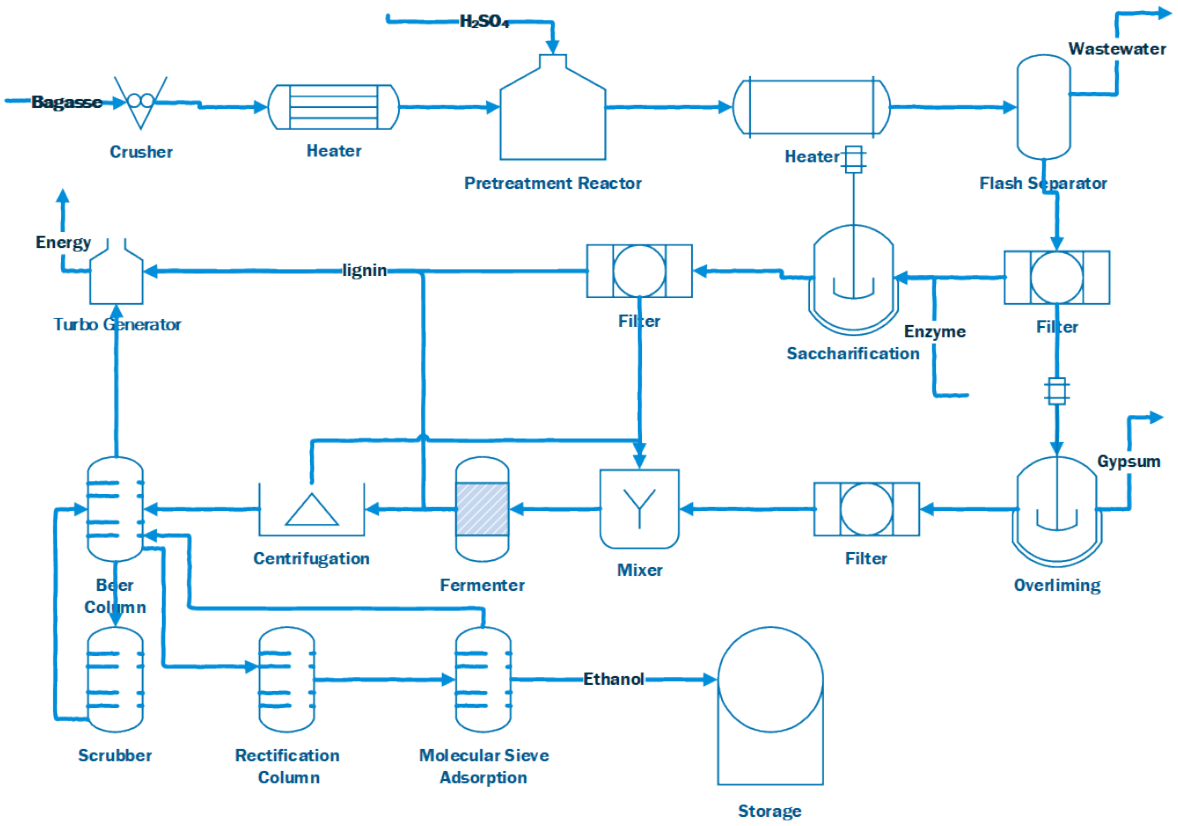


Figure 15 PFD for bioethanol production from sugarcane bagasse-based biorefinery plant, layout using Microsoft Visio

4.3 PROCESS DESIGN DESCRIPTION AND SIMULATION

After the data that helps to conceptually design the process were collected, the overall biorefinery plant was described and simulated in Aspen Plus simulation software. The conceptual design and simulation were prepared in a module wise. The superstructure biorefinery plant encompasses different modules. The biorefinery process consists: (1) pretreatment, (2) saccharification, (3) fermentation, (4) distillation and CHP units. The tasks of each module are presented in quantized manner. The data generated from one module was used as a feed for the next module.

The process modeling and simulation helps to identify potential improvements as well as possible difficulties. Although there are so many different types of commercial process simulating software, this simulation process is done in Aspen plus version 11. The mathematical model and other related financial calculation were also performed with the help of Matlab and Microsoft Excel. Aspen Plus software was written to solve the mass and energy balances and to calculate the thermodynamic properties of the streams involved in the process. The physical-property data for the components were obtained either from Aspen plus databank or from NREL's databank on biomass for wood components such as cellulose

and hemicellulose (Wooley & Putsche, 1996). The plant is assumed to be capable of processing 2000 dry tons of sugarcane bagasse per day which is the same for all the process configurations studied.

4.3.1 Feedstock Handling

Some of the mechanical operations performed in feedstock handling includes bale delivery, yard storage of sugarcane bagasse followed by milling and washing. The handling considers moisture (Grinder throughput, Particle size variability and Variation causes inconsistent mass and heat transfer in conversion), Particle Size (large particle not to cause plugging and fine particle not to cause dust fire, explosion, buffering capacity) and removing foreign material. The feedstock used for this biorefinery plant design is sugarcane bagasse, which is to be purchased from sugar factories. The chemical composition of typical bagasse is collected from authorized sources.

Table 4 Typical Sugarcane Bagasse Composition(Gao et al. 2013)

Total Amount of Bagasse		2000000 kg/h
Proximate analysis		
Parameters	Mass fraction (%)	Weight (kg/h)
Moisture	50	1000000
Ash	3.2	64000
Volatile matter	83.65	1673000
Fixed carbon	13.15	263000
Ultimate analysis		
Element	Dry weight (%)	Weight (Kg/h)
C	45.38	907600
H	5.96	119200
O	45.21	904200
N	0.15	3000
Chemical composition		
Component	Dry Weight (%)	Weight (Kg/h)
Cellulose	45	900000
Hemicellulose	25	500000
Lignin	20	400000
Extractives	6.8	136000

Source: Gao, Y., Xu, J., Zhang, Y., Yu, Q., Yuan, Z., Liu, Y., 2013. Effects of different pretreatment methods on chemical composition of sugarcane bagasse and enzymatic hydrolysis. Biores. Technol. 144, 396–400; De Medeiros, E.M., Posada, J.A., Noorman, H., Osseweijer, P., Filho, R.M., 2017. Hydrous bioethanol production from sugarcane bagasse via energy self-sufficient gasification-fermentation hybrid route: simulation and financial analysis. J. Cleaner Prod. 168, 1625–1635.

At the plant gate, the feedstock size was in the range of 2-5 mm length. With that size, the daily feed with uniform particle size distribution is 2,000 metric tonnes of bagasse. In addition to that, about 50% water was mixed to the bagasse. The overall compressed

procedure used in simulating the feedstock handling module. All the chemical components of the pre-processed bagasse were registered into or activated from the database library. Two sub streams named conventional Inert Solids (CI Solids) and mixed were created to channel the solid and liquid components.

4.3.2 Acidic Pretreatment

After the feedstock bagasse is handled, same size of feedstock was assumed provided into the plant throat. The main purpose of the pretreatment module was to disclose and make susceptible the lignin part of the bagasse. The pretreatment process converts most of the hemicellulose carbohydrates in bagasse to soluble sugars (xylose, mannose, arabinose, and glucose) by hydrolysis reactions. Acetyl groups in the hemicellulose were liberated as acetic acid. The breakdown of biomass in pretreatment facilitates downstream enzymatic hydrolysis by disrupting cell wall structures, driving some lignin into solution, and reducing cellulose crystallinity and chain length. The nature and extent of such changes were highly dependent on the pretreatment chemistry and reaction severity (defined by residence time, temperature, and catalyst loading). Sugar degradation products such as furfural and 5-hydroxymethyl furfural (HMF) can also be formed in pretreatment.

The procedures, which have been used in simulating the acidic pretreatment stage were briefed here under. First, about 2000 tonnes of milled uniform particle size distributed sugarcane bagasse was fed into a mixer. Sulfuric acid and 100^{o}_{c} of water were mixed with the feedstock. After heating the mixture, acidic pretreatment starts in a separate reactor with about 13 atm pressure steam. Using blowdown tanker, the main intermediate product was separated from the waste water. Then, over liming and reacidification will continue with separate reactors. Finally, the result of the acidification process will feed into the saccharification stage.

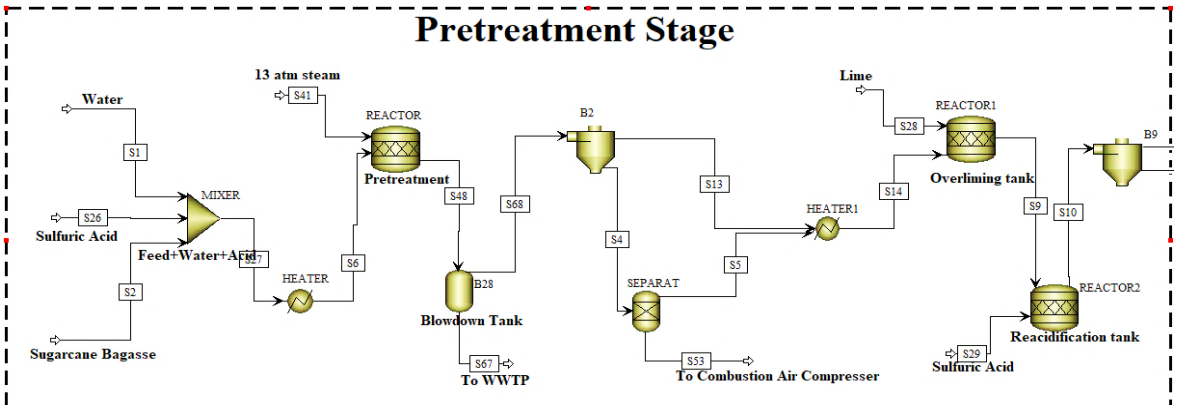


Figure 16 Process flow diagram of pretreatment stage, Aspen Plus V11

4.3.2.1 Chemical Changes During Acidic Pretreatment

The diluted sulfuric acid pretreatment module results a chemical and physical changes on the feedstock, bagasse. By referring different experimentally conducted and officially published literatures, the main physical and chemical changes, which has occurred during pretreatment are listed in an equation below. The main reaction during pretreatment was hydrolysis reaction. This means, addition of water to the polymers makes to dissociate and result a monomer or oligomer of the polymer. All the rate of reaction was assumed as first-order reaction.

Equation 3 Chemical reaction equations involved in sugarcane bagasse acidic pretreatment(Alvarado-Morales et al. 2009)

Chemical Reaction Equations	Conversion (%)
Hemicellulose + water ==> xylose	90%
Hemicellulose ==> furfural + 2water	5%
Cellulose + water == > glucose	7%
Acetate == > acetic acid	100%

Source: Alvarado-Morales, M., Terra, J., Gernaey, K.V., Woodley, J.M., Gani, R., 2009. Biorefining: computer aided tools for sustainable design and analysis of bioethanol production. Chem. Eng. Res. Des. 87, 1171– 1183; Aden, A., 2002. National Renewable Energy Laboratory (U.S.).

The above table indicates the result of acidic pretreatment. The acidic pretreatment converts some of the main components of bagasse into another easily accessible form of products. For instance, hemicellulose had converted into xylose and furfural at 90% and 5% respectively.

4.3.3 Simultaneous Saccharification and Co-fermentation (SSCF) Reactions

Fermentation is the heart of biochemical this biorefinery processing plant. It is a process of converting bagasse components into valuable products with the help of microorganism. Those microorganisms need specific working condition. The first stage on the biochemical conversion is saccharification. At saccharification, conditions were adjusted to host the cellulase enzyme. In here all the celluloses were expected to be converted from cellulose into glucose. The second biochemical reaction was fermentation. The saccharification and fermentation process took at the same stage. The stage simulation procedure were highly condensed and presented as follow.

The result of acidic pretreatment was feed into a saccharification reactor. In the same reactor cellulase broth and enzyme were added. After adjusting proper condition for some times, the result of saccharification, corn steeper liquor and diammonium phosphate were mixed into

one separate seed reactor. The feed reactor was located prior to fermentation stage. The product of seed fermenter was split into side reaction reactor and main reaction reactor. Side reactor was simulated for contaminants. Then, the result of the two fermenters reunite as fermentation broth. After heating the fermentation broth, the next distillation process continuous.

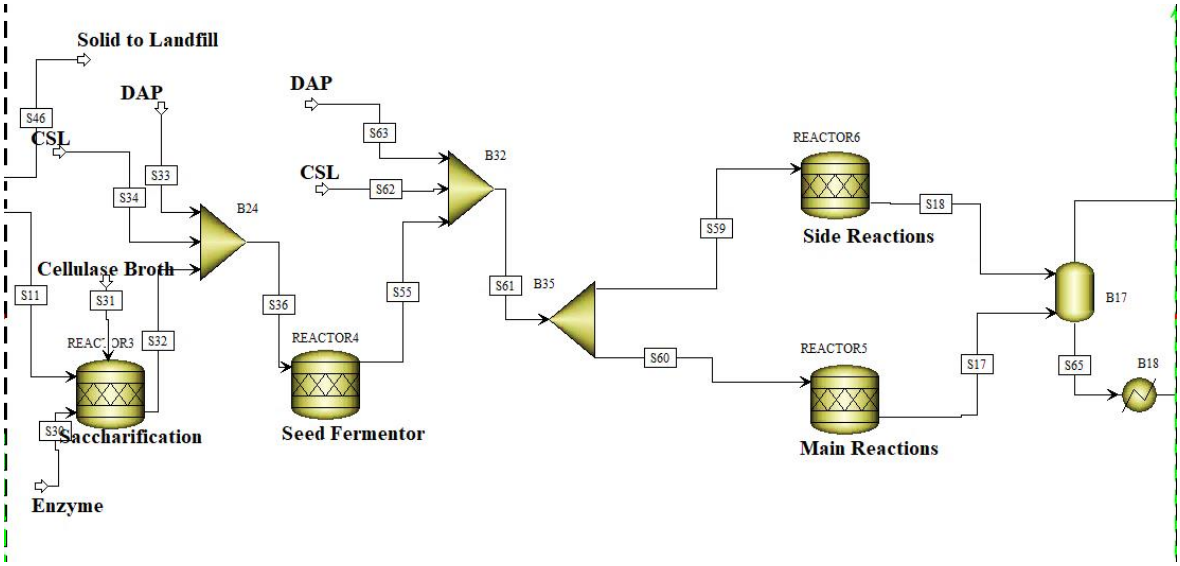


Figure 17 Process Flow Diagram of Saccharification and fermentation stages({Aspen Technology 2000)

4.3.3.1 Saccharification Operating Condition

Saccharification was performed biochemically. Those condition were adjusted in favor of the enzyme and microorganism' important conditions. In this biochemical conversion process, the enzyme was assumed produced on-site. The reaction operates at 48^{o}_{c} for about 3.5 days (Humbird 2011). For 0.2% of total solid concentration, 19.9 mg/g cell concentration of enzyme was loaded(Sherief, El-Naggar, and Hamza 2010).

4.3.3.2 Saccharification Chemical changes

The enzymatic hydrolysis is a type of biochemical reaction supported with enzyme and water. During the enzymatic hydrolysis, some chemical and physical changes were occurred. Those chemical and physical changes are formulated in chemical reaction equations by different scientist. By referring different literatures from around the world, the most important chemical equation is listed in the equation below.

Equation 4 Chemical reaction equation occurred during saccharification process of cellulose

Chemical Reaction Equation	Conversion (%)
Cellulose + water == > glucose	90%
Cellulose + 0.5water == >0.5cellobiose	1.2%

Cellobiose + water == > 2glucose	95%

4.3.3.3 Saccharification Mathematical Modeling

The above chemical changes were occurred due to water and cellulase enzyme. Depending on the above chemical reaction, the reaction kinetics of the cellulase enzyme are formulated mathematically by different researchers. One of the most common models used to mathematically express the saccharification was developed by (Kadam, Rydholm, and Mcmillan 2004). According the equation written in equation 4, the decomposition of cellulose to cellobiose (eq. 22) and glucose (eq. 23) by the action of the enzyme's endo-β-1,4-glucanases + exoglucanases; (2) cellobiose hydrolysis into glucose by β-glucosidase enzyme activity (eq. 24). The model furthermore describes enzyme adsorption (eq. 25), the concentrations of free and bound enzyme (eq. 26), substrate reactivity (eq. 27) and the effect of the temperature on the saccharification by means of the Arrhenius equation (eq. 28).

Equation 5 Saccharification Mathematical Modeling(Kadam et al. 2004)

Cellulose to Cellobiose	$r_1 = \frac{K_{1r} C_{E_{1B}} R_S C_S}{1+\frac{C_{G_2}}{K_{1IG2}}+\frac{C_G}{K_{1IG}}+\frac{C_{xy}}{K_{1Ixy}}}$	[22]
Cellulose to Glucose	$r_2 = \frac{K_{2r} C_{E_{1B}} + R_S C_S}{1+\frac{C_{G_2}}{K_{2IG2}}+\frac{C_G}{K_{2IG}}+\frac{C_{xy}}{K_{2Ixy}}}$	[23]
Cellobiose to Glucose	$r_3 = \frac{K_{3r} C_{E_{2f}} C_S}{K_{3M}(1+\frac{C_G}{K_{3IG}}+\frac{C_{xy}}{K_{3Ixy}}) + C_{G2}}$	[24]
Enzyme Adsorption	$E_{iE/B} = \frac{E_{imax} K_{iad} C_{E_{iF}} C_S}{1+K_{iad} C_{Eif}}$	[25]
Enzyme	$E_{E_{f1}} = C_{E_{f1}} + E_{E_{f1}}$	[26]
Substrate Relativity	$R_S = \alpha \frac{C_S}{S_0}$	[27]
Temperature Dependence	$K_{tr(T2)} = K_{tr(T2)} e^{\frac{-E_a}{R}(\frac{1}{T1}-\frac{1}{T2})}, 30_c^o \leq T \leq 55_c^o$	[28]

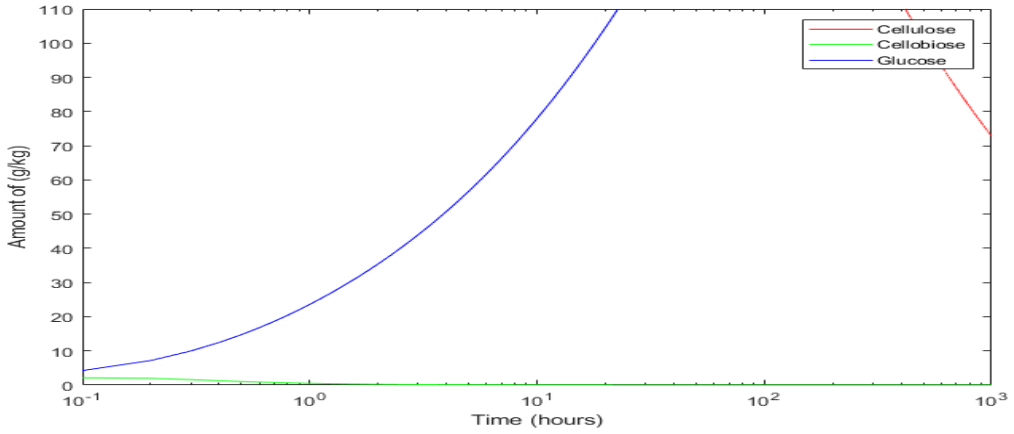


Figure 18 Saccharification process plotted in Matlab(Documentation 2012)

4.3.3.4 Co-fermentation Operating Condition

Following the saccharification process, the co-fermentation reaction was activated. Although there is also another separate method of fermentation, co-fermentation was chosen for this model. This is because the availability of a strain, Z.mobilis ZM4 (pZB5) that able to ferment both pentose (C_5) and hexose (C_6) sugars at the same time(Majidian et al. 2018). Since the types of strain used for this co-fermentation method was different from saccharification, the condition is also different.

Table 5 Co-fermentation operating condition(Humbird et al. 2011)

Fermenter Parameters	**Values**
Total Solids (wt%)	0.198
Insoluble Solids (wt%)	0.051
Temperature (°C)	32
Pressure (atm)	1
Residence Time (days)	1.5
Inoculum level	10 vol% of production vessel size
Batch time	24h
Fermenter turnaround time	12h
Number of trains	2
Number of fermenter stages	5
Maximum fermenter volume	757m cubic
Corn steep liquor (CSL) loading	0.5 wt%
Diammonium phosphate (DAP) loading	0.65 g/L fermentation broth

4.3.3.5 Co-fermentation Chemical Reactions

During cofermentation biochemical and physical changes were occurred. The reactant for the biochemical changes were commonly glucose and xylose sugars. The process of converting from reactant to product, ethanol and other byproducts was with the help of Z.mobilis ZM4 (pZB5)(Singh and Harvey 2009).

Equation 6 Co-fermentation biochemical reaction equation(Singh and Harvey 2009)

Chemical Reaction Equations	Typical Conversion (%)
Glucose	
Glucose == > 2EtOH + 2CO2	90%
Glucose + 2water == > 2glycerol + O2	0.5%
Glucose + 2CO2 == > 2succinic acid + O2	0.6%
Glucose == > 3acetic acid	1.5%
0.55 Glucose == > 0.33yeast + 1.11water + 0.45CO2	2%
Xylose	
3Xylose == > 5EtOH + 5CO2	85%
3Xylose + 5water == > 5glycerol + 2.5O2	0.3%
Xylose + water == > xylitol + 0.5O2	4.6%
3Xylose +5CO2 == > 5succinic acid + 2.5O2	0.9%
2Xylose == > 5acetic acid	1.4%
0.66Xylose == > 0.33yeast + 1.11water + 0.45CO2	4%

4.3.3.6 Co-fermentation Mathematical Modeling

The mathematical model employed in this work for the cofermentation part in the SSCF model has been adapted from (Hari Krishna, Janardhan Reddy, and Chowdary 2001), and considers the simultaneous conversion of xylose and glucose to ethanol, also known as a cofermentation. The cofermentation model was based on the Z. Mobilis. There were so many mathematical models out there. This mathematical model(Hari Krishna et al. 2001) is selected due the incorporation of product inhibitions. The mathematical model for cofermentation involves the reaction rates for: (1) cell growth on glucose (eq. 29) and xylose (eq. 30); (2) the total yeast cell mass production as the average product of the cell growth on glucose and xylose using the mass fraction of these compounds present in the mixture (eq. 31); (3) consumption of glucose (eq. 32) and xylose (eq. 33); (4) formation of ethanol from glucose (eq. 34) and xylose (eq. 35); (5) overall formation of ethanol (eq. 36).

Cell growth on glucose

$$r_1' = \left[\frac{\mu_{max1}.s_1}{K_1 + s_1 + s_1.\frac{k_1'}{k_2'}}\right].f_5(s_2+s_1).f_6(p) \quad [29]$$

Cell growth on xylose

$$r_2' = \left[\frac{\mu_{max2}.s_2}{k_2' + s_2 + s_2.\frac{k_2'}{k_1'}}\right].f_7(s_2+s_1).f_8(p) \quad [30]$$

Average product of the cell growth on glucose and xylose

$$\frac{dx}{dt} = r_1' + r_2' - D.X \quad [31]$$

Consumption of glucose

$$r_1 = x.\left[\frac{q_{max1}.s_1}{k_2' + s_2 + s_2.\frac{k_2}{k_1}}\right].f_1(s_2+s_1).f_2(p) \quad [32]$$

Consumption of xylose

$$r_2 = x.\left[\frac{q_{max2}.s_2}{k_z + s_2 + s_1.\frac{k_2}{k_1}}\right].f_3(s_2+s_1).f_4(p) \quad [33]$$

Formation of ethanol from glucose

$$\frac{ds_1}{dt} = -r_1 + D.(s_1^0 - s_1) \quad [34]$$

Formation of ethanol from xylose

$$\frac{ds_2}{dt} = -r_2 + D.D.(s_2^0 - s_2) \quad [35]$$

Overall formation of ethanol

$$\frac{dp}{dt} = r_1 + {Y_p}/{s_1} + r_2.{Y_p}/{s_2} - D.P \quad [36]$$

Subjected to

$$f(\varphi) = \{\alpha_i.\varphi^2 + b_i.\varphi + 1, f(\varphi) \geq 0\}\ \forall\ \varphi \in \{P, s_1 + s_2\}, i = 1,2,\ldots,8$$

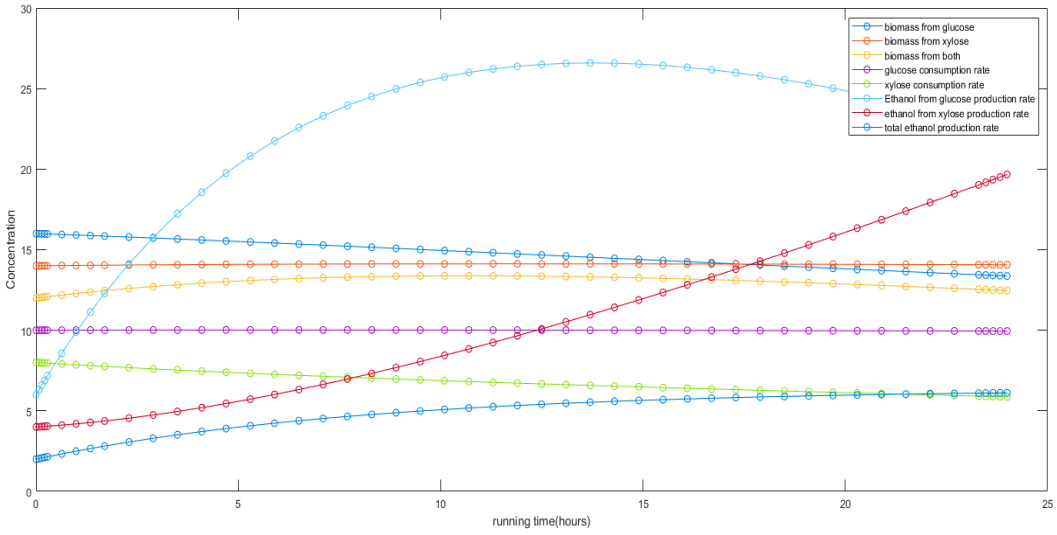


Figure 19 Mathematical model for Co-fermentation reaction plotted in Matlab(Documentation 2012)

4.3.4 Product Recovery Through Distillation Method

Although there were some by products due to the side reaction, ethanol is the main product of this biorefinery plant. At the end of the co-fermentation, ethanol in the form of fermentation broth was collected. The best technique chosen to separate ethanol from water was distillation followed by molecular sieve adsorption(Humbird et al. 2011). Rigorous Fractional (Radfrac) distillation column was the type of distillation column selected for the simulation. The procedures used to simulate this distillation module were. The fermentation broth was filtered using the lignin separator to separate the unconverted solid and lignin. The solid part sent to combustion for power generation. The CO_2, produced during fermentation was sent to the wet scrubber. The liquid part or beer was sent to the first distillation column (beer column). Then, the concentrated beer passed through the second distillation column to get overall concentration up to 92.5%. Finally, the process passes through vapor-phase molecular sieve adsorption to upgrade the concentration up to 99.5%.

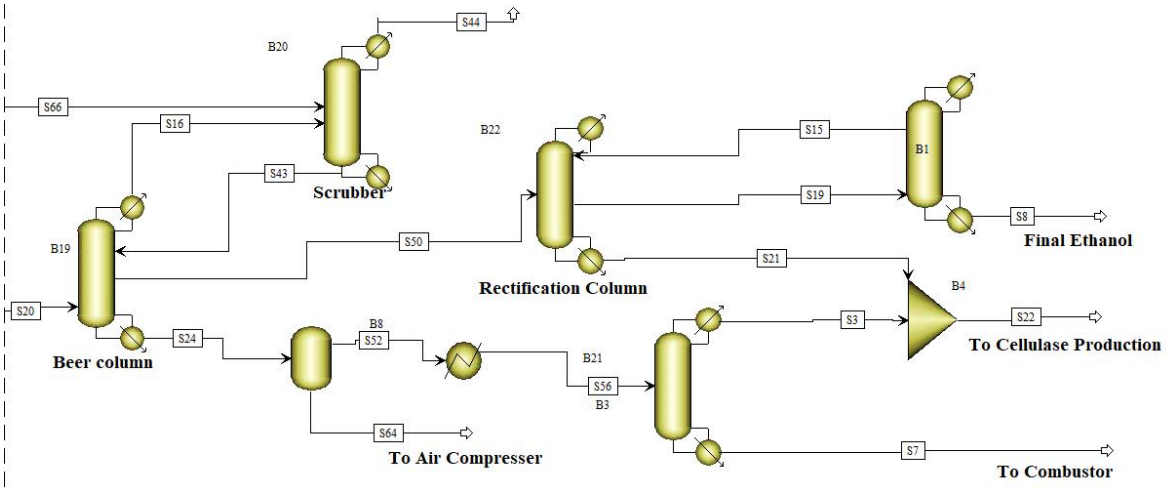


Figure 20 Process Flow Diagram of product, ethanol recovery stage

Figure 21 Beer and Rectification distillation column specification({Aspen Technology 2000)

Specification	Beer Column	Rectification Column
Trays	32	45
Tray efficiency (%)	48	76
Feed ethanol composition(wt%)	3.2	43.1
Draw ethanol composition (wt%)	39.2	92.5
Reboiler duty(kj/h)	$1.844*10^8$	$9.277*10^6$
Condenser duty (kj/h)	$8.600*10^7$	$4.887*10^7$

From the distillation column, the hydraulic plot was taken. Each individual distillation column stage has its own hydraulic plot. The plot varies depending on the hydraulic internal column analysis. The status of the hydraulic plot indicates as healthy. One of the representative internal column hydraulic plot is shown below.

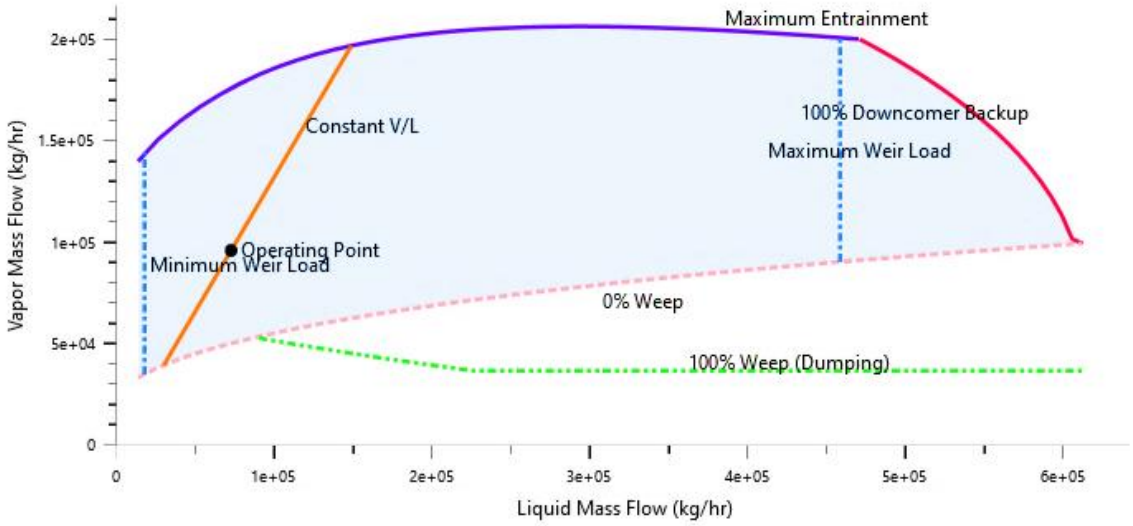


Figure 22 Distillation column Hydraulic plot, generated by Aspen Plus v 11(Aspen Technology 2000)

4.3.5 Process Design and Simulation Validation

4.3.5.1 The SSCF Mathematical Model Validation

The two mathematical model used for saccharification and co-fermentation were taken from authorized and published papers. Validation of the mathematical model by comparing with experimental data is important. The above mathematical modeling (Hari Krishna et al. 2001)(Kadam et al. 2004) of biochemical reaction kinetics used for SSCF was tested in Matlab. The source of data was retrieved from (Leksawasdi, Joachimsthal, and Rogers 2001). These two researchers use recombinant Zymomonas Mobilis to produce ethanol from glucose/xylose mixtures. For more details information about the experimental result (Leksawasdi et al. 2001).

4.3.5.2 Validation of Distillation Methods

Distillation method is one of the most important steps in the downstream process. The design and configuration of distillation column is very crucial to increase separation efficiency. There are experimental data to confirm the separation efficiency of water and ethanol. One of the best experimental data used for this ethanol recovery method was retrieved from the software database library. National Institute of Science and Technology (NIST) was also used as a source of thermodynamic data evaluation method for calibration and validation. The thermodynamic data engine was developed by (Dr. Kenneth, 2019).

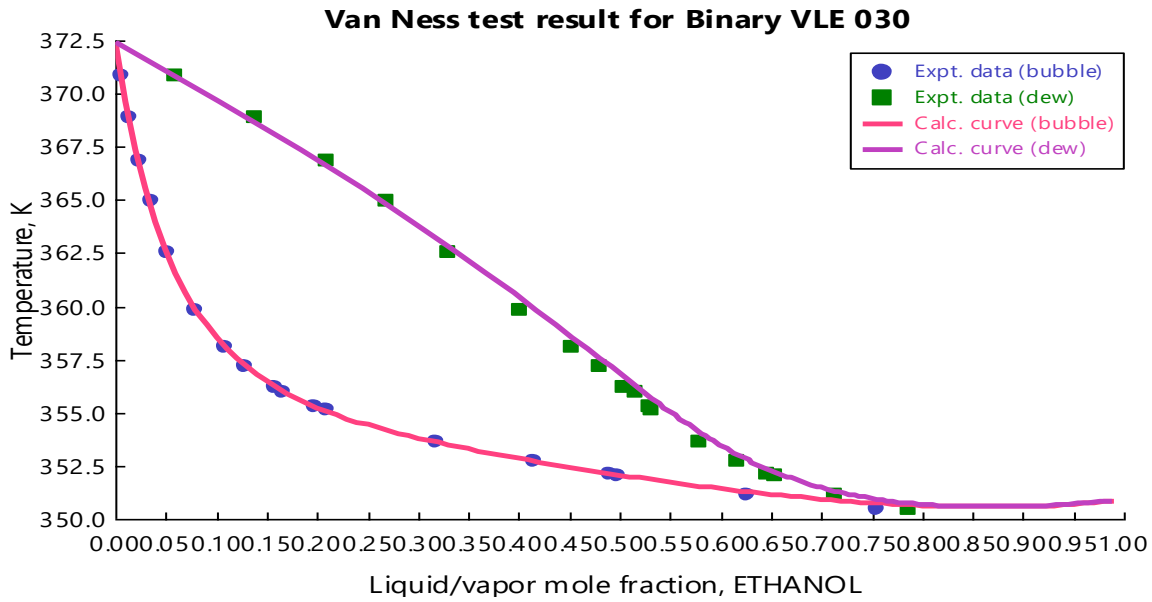


Figure 23 Liquid/vapor mole fraction of ethanol and water

The above figure depicts ethanol–water separation curve. It was a comparison of observational with the simulation data. The azeotropic point lays at about 78% ethanol liquid/vapor mole fraction with positive regression. As the experimental data shown green and blue color dots, they both overlay on the same line with the simulation. Therefore, the procedure used to simulate for the product recovery is indirectly validated.

CHAPTER 5: **TECHNO-ECONOMICS ANALYSIS**

5.1 FEEDSTOCK PLANT GATE COST ESTIMATION MODEL (FCEM)

The sugarcane bagasse was used as feedstock for this biorefinery plant. It was assumed, purchased from sugar factories. Although factories were considered the main source of bagasse, some individuals suppliers can also supply. Considering those individuals and sugar factories, overall cost of bagasse at the plant gate is estimated. In the cost estimation, profit of the supplier or the agent (farmer) was also considered. The major cost intensive activities, which are considered for this model were feedstock cost on its factory, labor and transport and crushing machinery cost, pre-processing cost, fuel cost, maintenance, and other related costs.

Table 6 Feedstock plant gate cost breakdown

S/No	Feedstock handling cost breakdown	Symbolic Representation
1	Cost for feedstock at factory field	C_{1n}
2	Cost for collection & transportation to storage	C_{2n}
3	Cost for primary processing & storage	C_{3n}
4	Cost for transportation into plant gate	C_{4n}

Table 7 Input data for different parameters used for feedstock cost estimation

Code	Parameters	Values	References
β_{cp}	Ratio of Actual Road to Direct Distance	0.65	Survey
t_{cp}	Fuel Cost Per Unit Distance & Unit Mass	$.25 /Truck	Survey
S_{cp}	Distance from Collection center to the processing facility	19.5 Km	Calculated
Q_{ncp}	Transport Quantity from collection center n to the processing facility	1tonne	Assumption
C_{lcp}	Cost of labor for transportation	$7/truck	Estimation
C_{decp}	Equipment Depreciation Costs	$2.25	Survey
C_{mcp}	Cost of equipment maintenance	$3.25	Survey
C_{ec}	Energy cost	$12/truck	(Zhao et al.2015a)
C_{lc}	Labor Cost	$3.5/tonne	Survey
C_{dmc}	Depreciation Cost of building & Equipment	$2.5	Survey

C_{landc}	Land Rent for the plants	$0	Survey
Y_n	Feedstock yield per unit area (hectare)	$.75tonnes/	Survey
αn	Fraction of useful land	.34	(Dutta et al. 2010)
R_n	Radius of collection	5 km	Survey
C_{lfc}	Product rate labors payment	$3	Estimation
C_1	Cost of bagasse from factory	$8/tonne	(Kazi, et.al., 2010)

By taking some important assumptions, the overall feedstock plant gate cost is estimated with the following equation.

Equation 7 Feedstock Cost Estimation Equations(Zhao et al. 2015)

$$Plant\ Gate\ Feedstock\ Cost\ (C = \sum_{j=1}^{4}\sum_{n=1}^{N} Cjn\ +\ P) \qquad [37]$$

where, C is the final plant-gate cost of feedstock; N is the number of all collection centers; n is the symbol of specific collection center; j is the symbol of each phase, namely at field, field-to-center, at center, and center-to-plant; and P is the profit of the agent

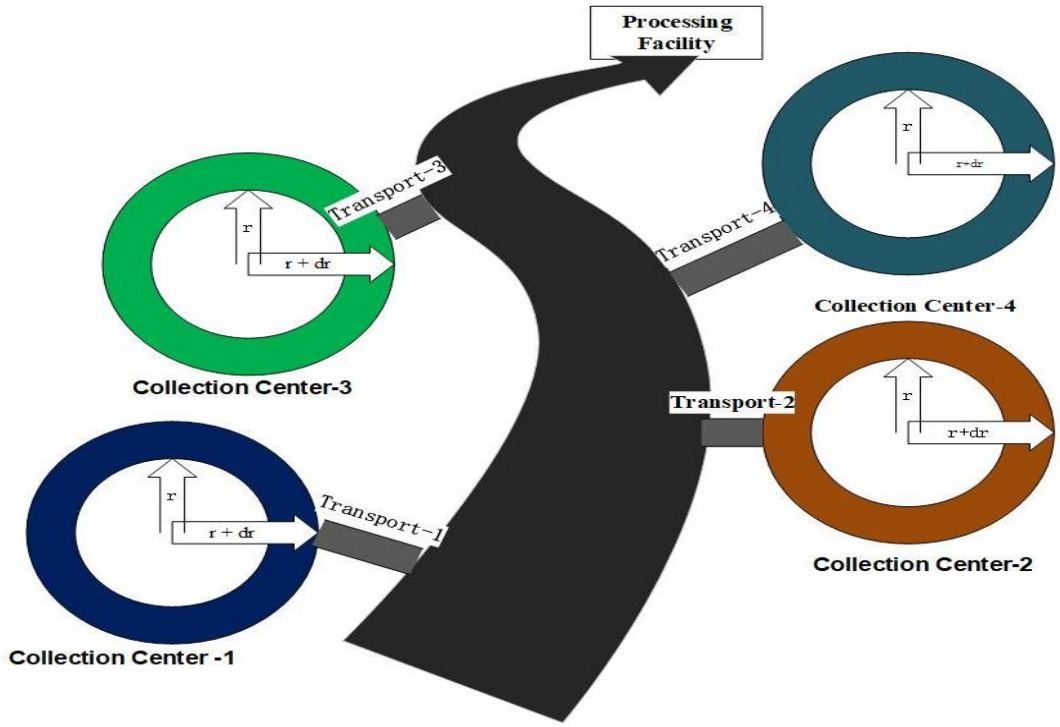


Figure 24 Feedstock cost estimation model

Cost of feedstock (C_n): the feedstock that was used by the biorefinery plant was collected from sugar factories. So, the cost of bagasse on its factory field is estimated.

Factory to center transport cost (C_{2n}): Factory to center transportation cost is the cost before storage and processing. In this stage, the cost of labor and machineries was

considered. The information about this was collected from online and local market survey, observation and some of them were incorporate with some estimation(Teka 2007). Therefore, the phase specific equation to estimate the cost spent from sugar factory to collection center is:

$$C_{2n} = C_{lfc} + C_{dfc} + C_{defc} + C_{mfc} + C_{ffc} \quad [38]$$

$$C_{2n} = 3.5 + 4.5 + 2.5 + 3.5 + 0.063 = \$13.8126$$

Where:

- C_{lfc} is the cost of labor for feedstock collection
- C_{dfc} is the cost of labor for vehicle driving
- C_{defc} is the cost of equipment depreciation
- C_{mfc} is the cost of equipment maintenance and other expenses
- C_{ffc} is the cost of fuel

The calculation of C_{ffc} was based on Nguyen and Prince(Nguyen and Prince 2006), which is

$$C_{ffC} = \int_0^{Rn} 2\pi\gamma_n a_n \beta_{fC} t_{fc} r^2 dr = \frac{2}{3}\pi \mathrm{Y} n a_n \beta_{fC} t_{fc} R^3 n \quad [39]$$

$$C_{ffC} = \frac{2}{3} x\pi x.75x.34x.65x.25x(1.3134)^3 = \$0.063$$

Where; Y_n is feedstock yield per unit area; α_n is the fraction of useful land; β_{fc} is the ratio of actual road length to direct distance, taken as constant, which is denoted as the tortuosity factor; t_{fc} is fuel cost per unit distance and unit mass. R_n is the maximum collection radius for the specific collection center, which was estimated based on equation:

$$R_n = \sqrt{\frac{Q_n}{\pi\gamma_n a_n}} \quad ==> R_n = \sqrt{\frac{1.5}{\pi x.75x.34}} = 1.3134 \quad [40]$$

Where; Q_n is the feedstock volume required for collection center n.

Cost at the center (C_{3n})

$$C_{3n} = C_{ec} + C_{lc} + C_{dmc} + C_{landc} \quad [41]$$

$$C_{3n} = .75 + 3.5 + 2.5 + 0 = \$6.75$$

where, C_{ec} is energy cost; C_{lc} is labor cost; C_{dmc} is depreciation cost of buildings and equipment; and C_{landc} is land rent cost.

Center to plant cost (C_{4n})

$$C_{4n} = C_{lcp} + C_{decp} + C_{mcp} + C_{fcp} \quad [42]$$

$$C_{4n} = 7x2.25x3.5x3.1685 = \$15.91875$$

where C_{lcp}, C_{decp}, C_{mcp} and C_{fcp} are the costs of labor for transportation, equipment depreciation, and the cost of equipment maintenance and other expenses, and fuel cost respectively. C_{fcp} was calculated as:

$$C_{fcp} = Q_{ncp} S_{Cp} \beta_{Cp} t_{Cp} \quad [43]$$

$$C_{fcp} = 1x19.5x.65x.25 = \$3.1685$$

where Q_{ncp} is transport quantity from collection center n to processing facility; S_{cp} is transport distance from collection center n to the processing facility; βcp is the ratio of actual road length to direct distance, and t_{cp} is fuel cost per unit distance and unit mass from collection center to processing facility. Transport distance S_{cp} is calculated as

$$S_{Cp} = R_n x N \, x \, \beta_{Cp} \quad [44]$$

$$S_{Cp} = 5x6 \, x.65 = 19.5m$$

Profit of the agent (P): the profit of the agent (p) was assumed 5% of the total estimated cost(Zhao et al. 2015). The calculation was then estimated based on the recommendation from Nguyen and Prince (Nguyen and Prince 2006). The profit depends on the sum of C_{2n}, C_3n and C_4n as estimated below:

$$p = 5\% \, (C_{2n} + C_{3n} + C_{4n}) \quad [45]$$

$$p = 5\% \, (13.8126 + 6.75 + 15.91875) = \$1.824$$

Based on the above the plant gate feedstock cost estimation model, the cost of each tonne of biomass collected, preprocessed, and transported is:

$$(C = 8 + 13.8126 + 6.75 + 15.91875 + 1.824 = \$46.3054 \quad [46]$$

The cost of the feedstock at the plant gate is estimated in the above method and it is $46.3054 per tonne. This result is used in all the simulations. This value is compared with some already calculated values from around the world in the table below.

Table 8 Unit cost breakdown for woody biomass feedstock taken (Dutta et al. 2016)

Parameters	Pulpwood	Wood Residues	Switchgrass	Construction & Demolition	Bagasse cost
Grower payment	27.56	29.05	21.68	8.98	24.14
Harvest and Collection	24.52	0.00	16.99	0.00	11.54
Landing Preprocessing	13.42	9.62	0.00	10.86	11.29
Transportation	12	3.67	4.96	7.57	8.29
Preprocessing	26.42	26.42	21.72	31.00	27.19
Storage	3.56	3.56	6.06	3.56	3.64
Handling	2.09	2.09	2.09	2.09	2.09
Total cost, $/dry tonne	109.67	74.42	73.50	64.07	88.18

5.2 BIOETHANOL PLANT-GATE PRICE ASSESSMENT MODEL (BPAM)

Bioethanol plant-gate price assessment model is part of the techno-economic analysis, which summarizes the capital investment and operating costs. This model is developed to fit market condition depending on the NREL 2012 design repot(Davis et al. 2015).

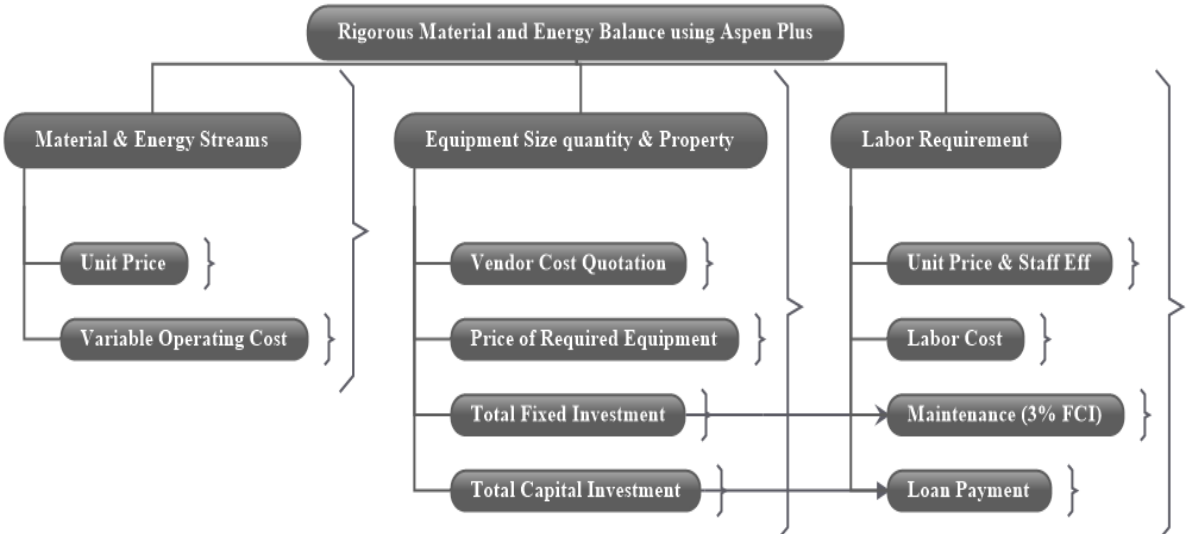


Figure 25 Flowsheet diagram for rigorous material and energy balance using aspen plus

The above model of technology pathway, energy, and material balance were described using Aspen Plus version 11. The simulation performs those all tasks using some built-in mathematical model function. The total capital investment (TCI) was computed based on the

total equipment cost using the Langer coefficient method(Modenbach and Nokes 2013). The variable operating costs (VOC) were determined based on material and energy data produced by simulation and quoted unit prices of the material and energy. Fixed operating costs (FOC), including labor costs, maintenance, and management expenses, were determined based on factors such as the scale of the plant, fixed capital investment (FCI), TCI, and annual sales. Taxes were determined in line with federal tax regulations. With these costs, the paper used a discounted cash flow analysis to determine the PGP of ethanol required to obtain a zero net present value (NPV)(Zhao et al. 2015) with a finite internal rate of return as shown in formula below.

Equation 8 Net Present Value calculation equation(Zhao et al. 2015)

$$NPV = \sum_{t=2}^{30} \frac{PGP_t + Q_t + Pb_t - F_t - Mc_t - Loan_t - T_t}{(1+IRR)^t} = 0 \quad [47]$$

where:

TC_I is the initial total capital investment;

t is the year of plant operation, and construction lasts for 3 years,

PGP_t is plant-gate price of ethanol product in year t;

Q_t is ethanol production in year t;

Pb_t is the price of the byproduct (excess electricity) in year t;

Qb_t is the production of the byproduct in year t;

Ft is feedstock cost in year t;

Mc_t is the operating cost of ethanol in year t;

$Loan_t$ is the loan payment (including interest) in year t;

T_t is the taxes paid by the plant in year t;

To estimate the minimum ethanol selling price, the major cost contributors must be determined first. Those major cost contributors are total capital investment, variable operating cost, and fixed operating costs. Those major cost contributors were estimated using the simulation software.

5.2.1 Total Capital Investment

The investment cost of the plant was the cost of equipment used to erect the biorefinery plant. That equipment was sized to fit the required volume and shape. Based on the volume increment and decrement, the cost was calculated using the cost index of chemical engineering plant cost index, which is attached in appendix. The cost of the equipment is calculated in dollar, which is the software's default currency. Each piece of equipment has a purchased cost that reflects a quote made in a certain year. Capital costs provided by Harris Group in 2014 or 2015 were adjusted using the Plant Cost Index from Chemical Engineering Magazine to a common basis year of 2016. However, the sizing and equipment type selection and evaluation is performed by the software. Similarly, for chemical costs I used the Industrial Inorganic Chemical Index from SRI Consulting, which is also referred in appendix. To estimate the cost of equipment or chemicals for present time and at project location, different cost estimation mechanisms were used by the software.

Equation for effect of size (Capacity): $\frac{C_a}{C_b} = \left(\frac{A_a}{A_b}\right)^n$ [48]

Where: A = Equation cost attribution

C = Purchased cost

N = Cost exponent

Subscription: a refers to equipment with required attribute

b refers to equipment with the base attribute

Equation for time effect: $C_2 = C_1\left(\frac{I_2}{I_1}\right)^n$ [49]

Where: C= is purchasing cost and I =is cost index

Subscription: 1 refers to base time when cost is known

2 refers to time when cost is desired

n is a characteristic scaling exponent (typically in the range of 0.5 to 0.7)

The total capital investment was estimated by considering the time and capacity factors. Once the total installed equipment cost has been determined in the year of interest, the direct, indirect, fixed capital investment ($184,534,014), working investment ($9,226,700.70) and land ($1,007,049) was adding up to total capital investment (TCI) of $195267764. One of the cost factors added by the software was distance factor, development, and warehouse

costs. Those costs were based on the inside-battery-limits (ISBL) equipment costs (Module 200, 300, 400, and 500) and are considered part of the total direct cost (TDC) ($122,640,618). Project contingency, field expenses, home-office engineering and construction activities, and other costs related to construction were computed relative to the TDC and give the fixed capital investment (FCI). The sum of FCI and the working capital for the project is the TCI. Based on the recommendation from Harris Group, the equipment vendor, home office and construction charge 20%. The Contingency was charged 10% of the TDC.

Table 9 Summary of biorefinery plant cost, generated from Aspen plus v10

Parameters		Description	Amount
Total equipment purchased cost, TEPC			$57,296,300
Equipment installation	40%	of TEPC	$22,918,520
Instrumentation and control system	13%	of TEPC	$7,448,519
Process piping	31%	of TEPC	$17,761,853
Electrical equipment	10%	of TEPC	$5,729,630
Buildings	10%	of TEPC	$5,729,630
Site development	10%	of TEPC	$5,729,630
Total plant direct cost, TPDC			$122,614,082
Engineering design and supervision	32%	of TEPC	$18,334,816
Construction	34%	of TEPC	$19,480,742
Total plant indirect cost, TPIC			$37,815,558
Total plant cost, TPC			$160,429,640
Contractor’s fee	5%	of TPC	$8,021,482.00
Contingency	10%	of TPC	$16,042,964.00
Operating Cost			$221,232,000.00
Fixed capital investment, FCI			$184,494,086
Working capital	5%	of FCI	$9,224,704.30
Land			$1,007,049
Total capital investment, TCI			$194,725,839

5.2.2 Operating Costs

5.2.2.1 Fixed operating cost (FOC)

Fixed operating costs are generally costing payed off despite the plant fully working or not. Most common list of fixed operating costs are labor and various overhead items. The hardest part of this section was specifying how much number of labors was required. To decide the labor number, referring similar design report was very important. So, the type of required quality and number of labors by the same quality were taken from techno-economic analysis of similar report(Zhao et al. 2015). However, the amount of salary was specified based on the survey in the local market, some authorized online websites, and some estimation with the help of my advisor, Dr. Ing Hundessa Desalegn. One of the labor-intensive modules of the plant, feedstock handling is outsourced to an agent.

Table 10 Fixed Operating cost of employees of the biorefinery plant: Source: Salaryexplorer.com

Position	Monthly Salary ($/m)	Annual Salary ($/y)	# Required	Subtotal (S/y)
Plant Manager	$ 346.23	$ 10,387.00	1	$ 10,387.00
Plant Engineer	$ 239.30	$ 7,179.00	2	$ 14,358.00
Maintenance Supervisor	$ 275.03	$ 8,251.00	1	$ 8,251.00
Maintenance Tech	$ 144.00	$ 4,320.00	15	$ 64,800.00
Lab Manager	$ 147.40	$ 4,422.00	1	$ 4,422.00
Lab Technician	$ 147.40	$ 4,422.00	2	$ 8,844.00
Lab Tech-Enzyme	$ 174.87	$ 5,246.00	2	$ 10,492.00
Shift Supervisor	$ 260.97	$ 7,829.00	12	$ 93,948.00
Shift Operators	$ 201.07	$ 6,032.00	75	$ 452,400.00
Sales manager	$ 431.33	$ 12,940.00	1	$ 12,940.00
Salesperson	$ 208.80	$ 6,264.00	6	$ 37,584.00
Yard Employees	$ 144.87	$ 4,346.00	6	$ 26,076.00
Clerks & Secretaries	$ 158.30	$ 4,749.00	3	$ 14,247.00
Grand Total Salaries	$ 2,879.57	$ 86,387.00	127	$ 758,749.00
Labor Burden (80%)	$ 5,183.22	$ 155,496.60		$ 1,365,748.20

Considering the federal taxation system, for each individual employee, 80% labor burden is applied to their salary. This labor burden covers safety, general engineering, general plant

maintenance, payroll overhead (including benefits), plant security, janitorial and similar services, phone, light, heat, and plant communications, payroll taxes, pension costs and health insurance. The 80% burden was taken from survey of related local and international companies. The percentage of cost for annual maintenance of equipment is 0.3% of installed cost(Davis et al. 2015).

5.2.2.2 Variable Operating Costs

The variable operating cost of the plant are those material costs which are imported or locally purchased. The inputs model and overall simulation was developed by NREL. One of the streams on the process modeling was material and energy cost of the plant. The materials are the groups of operating costs that must be purchased to run the plant. The materials were used at the different streams where they are required. Some of the materials were locally purchased and some of them are imported. The calculation of the stream estimates the calculation of for about a year. The estimated value is taken by calculating using index and by estimating through survey and reference.

Table 11 Raw material cost collected from online source (Balat 2011)

Material	**$/tonne**
Feedstock	$ 46.80
Sulfuric Acid, 93%	$ 81.39
Corn Steep Liquor	$ 51.55
Diammonium Phosphate	$ 895.32
Sorbitol	$ 1,021.93
Glucose	$ 526.52
Corn Steep Liquor	$ 51.55
Ammonia	$ 406.96
Host nutrients	$ 745.30
Sulfur Dioxide	$ 275.70
Caustic (as pure)	$ 135.65
Boiler Chems	$ 4,532.17
FGD Lime	$ 180.87
Cooling Tower Chems	$ 2,716.10
Makeup Water	$ 0.00

The above materials were listed by referring different literatures, survey local market, visiting some known online retailers and mainly from NREL 2016 design report. Most of the raw material have similar trends of increasing from previous year. The cost factors implemented for this design were the distance, time, and size effect.

5.3 CASH FLOW ANALYSIS

Cash Flow Analysis is the balance of total cash in and cash out. This mean the total cost in and generated revenue. This estimation was done after the total capital investment, variable operating costs, and fixed operating costs have been determined. Discounted cash flow rate of return (DCFROR) analysis is used to determine the minimum selling price per liter of ethanol produced. The discounted cash flow analysis was calculated by iterating the selling cost of ethanol until the net present value of the project was zero. To do this cash flow analysis the discount rate, depreciation method, income tax rates, plant life, and construction start-up duration be specified. In addition to the requirement, the loan term is also assumed due to the equity-financing system.

5.3.1 Discount Rate

The discount cash flow rate analysis is the rate for in and out flow of money. It was estimated depending on 30 years of plant life time. Based on that discount rate (which is also the internal rate of return [IRR] in this analysis) was set to 10%. Discount rate was also used in most similar biorefinery design reports and based on recommendation from Jang and Choi (Jang and Choi 2018) on how to perform economic evaluations of renewable energy technologies. Their view was that, In the absence of statistical data on discount rates used by industrial, transportation and commercial investors for investments with risks like those of conservation and renewable energy investments, it is recommended that an after-tax discount rate of 10% is used.

5.3.2 Equity financing

Equity financing for this analysis was assumed that the plant would be 50% equity financed. According the local and global financing institutes, the terms of the loan were taken to be 7% interest for 10 years. Developmental and commercial banks were under consideration for the source of 50% finance. The principal is taken out in stages over the 3-year construction period. Interest on the loan is paid during this period, but principal is not paid back.

5.3.3 Depreciation cost

Depreciation is the gradual decrease in the economic value of the capital firm. Depreciation of the biorefinery plant in terms of money is considered as cost. So, the depreciation cost must be calculated before or after tax. There are different methods to calculate depreciation cost. Straight line (SL) depreciation cost takes about 20 years to recover. The other method is modified accelerated cost recovery system. To determine the capital depreciation amount for the calculation of federal taxes to be paid, the IRS Modified Accelerated Cost Recovery System (MACRS) method was used. MACRS, system is the General Depreciation System (GDS), which allows both the 200% and 150% declining balance (DB) methods of depreciation. This offers the shortest recovery period and the largest tax deductions. According to IRS publication 946(USA-IRS, Revenue 2019), a cellulosic ethanol plant would fall under Asset Class 49.5, Waste Reduction and Resource Recovery Plants. This class uses a 7-year recovery period. IRS publication 946 contains a special provision for cellulosic biofuels plants that allows them to write off 50% of the capital investment in the first year(USA-IRS, Revenue 2019) . Although the provision affects the cash flow in the first few years of the analysis, it does not change the year in which the plant goes into the black and must start paying taxes.

5.3.4 Taxes

The federal corporate tax rate used for this analysis is 35%. Income tax is averaged over the plant life and that average was calculated in per-liter basis. The amount of income tax to be paid by a potential ethanol producer varies annually due to changes in the volume of product produced and the allowable depreciation deduction. Three-year tax-free taken as a global average for start-ups. This is because the depreciation and loan interest deductions are greater than the net income.

5.3.5 Construction Time

The construction time is important to the cash flow analysis because no income is earned during construction, but huge sums of money are being expended. Researchers indicate that small projects (less than $10 million investment) can be constructed in fewer than 18 months and that larger projects can take up to 42 months(Dutta et al. 2011). Certainly, this ethanol process is much smaller than a petroleum refinery, so using a construction time of 24 months fits within these references, although an important difference between this type of facility and a refinery is the large number of field-erected vessels. These are constructed on-site and

have a longer construction time than if the tanks were delivered finished. Twelve months are added before construction for planning and engineering.

Table 12 Time table for Project construction activities(Jang and Choi 2018)

Start month	End month	Activity Description	%Cost
0	12	Project plan and schedule established; conceptual and basic design engineering, permitting completed. Major equipment bid packages issued, engineering started on selected sub-packages, P&IDs complete, preliminary plant and equipment arrangements complete.	8%
12	24	All detailed engineering including foundations, structure, piping, electrical, site, etc. complete; all equipment and instrument components purchased and delivered; all site grading, drainage, sewers, rail, fire pond, foundation, and major structural installation complete; 80% of all major process equipment set (all except longest-lead items), all field fabricated tanks built, and most piping and electrical materials procured.	60%
24	36	Complete process equipment setting, piping, and instrumentation installation complete; all electrical wiring complete; all building finishing and plumbing complete; all landscaping complete; pre-commissioning complete; and commissioning, start-up, and initial performance test complete.	32%
		TOTAL	100%

5.3.6 Start-Up Time

Perry and Green (John H. Perry, Robert H. 2008) indicate that for a moderately complex plant, start-up should be about 25% of the construction time, or 6 months in this case. Delta-T's experience with start-up indicated that a large grain-to-ethanol plant could be started up in less than 6 months. Four months is selected to be a start-up time for this biorefinery plant. The start-up period is not completely wasted. However, it is expected that an average of 50% production could be achieved during that period while incurring 75% of variable expenses and 100% of fixed expenses.

5.3.7 Working Capital

Peters and Timmerhaus(M. S. Peters and K. D. Timmerhaus 1991) define working capital as money available to cover (1) raw materials and supplies in inventory, (2) finished product in storage, (3) accounts receivable, (4) cash on hand for monthly payments such as wages and maintenance supplies, (5) accounts payable, and (6) taxes payable. They indicate that working capital is usually 10%–20% of the fixed capital investment. This flow of money is required over the life of the plant, beginning in the start-up phase to make product that generates revenue to use in purchasing more materials and supplies. On-site ethanol storage capacity is 7 days; if the product is shipped, payment received in 30 days is conservative(Dutta et al. 2011). Therefore, a lower number seems reasonable. Garrett suggests that using a fraction of the yearly operating cost, typically 10%–35%, is more relevant. The total estimated working capital for this biorefinery plant is $9,226,700.70, or 5% of the fixed capital investment.

5.4 MINIMUM ETHANOL SELLING PRICE (MESP) ESTIMATION

Once the total capital investment, variable operating costs, and fixed operating costs have been determined, a discounted cash flow analysis was determined.

Table 13 Parameters used to determine the discount cash flow analysis

Items	**Design**	**Research Article**	**NREL Case**
Plant life	30 years	30 year	30 years
Discount rate	10%	13%	10%
General plant depreciation	200% declining balance (DB)	SL Depreciation	200% declining balance (DB)
General plant recovery period	7 years	20	7 years
Steam plant depreciation	150% DB	depreciation	150% DB
Steam plant recovery period	20 years	20 years	20 years
Federal tax rate	35%	35%	35%
Financing	50% equity	40% equity	40% equity
Loan terms	10-year loan at 7% APR	10-year loan at 6.9%	10-year loan at 8% APR
Construction period	3 years	3 years	3 years
First 12 months' expenditures	8%	8%	8%
Next 12 months' expenditures	60%	60%	60%
Last 12 months' expenditures	32%	32%	32%
Working capital	5% of FCI	5% of FCI	5% of FCI
Start-up time	4 months	3 Months	3 Months
Revenues during start-up	50%	50%	50%
Variable costs incurred during start-up	75%	75%	75%
Fixed costs incurred during start-up	100%	100%	100%
Feed-in tariff	$0.018/kwh	$0.123/kwh	

The discounted cash flow analysis is calculated by iterating the selling cost of ethanol until the net present value (NPV) of the project is zero. Some of the most important contributors for minimum ethanol selling price calculation are feedstock costs, enzyme production costs, non-enzyme conversion costs, feedstock handling cost, internal rate of return, equity percent

of total investment and others. The other most commonly used method of ethanol selling price calculation is using the breakeven point assumption(F.K, Kazi 2010). This is because the biofuel revenue (BR) from the sales of these ethanol is determined at the breakeven point where total revenues and total costs are equal. For the basic design, total revenues include the revenues generated from biofuel and excess electricity sales, whereas total costs include operating costs, return on investment and income tax. After performing a detailed power cycle analysis and by assuming the excess electricity is sold at 0.018kw/h, the electricity revenue (ER) from the excess electricity sales is found to be $excess\ electricity * tariff = 1.099 * 10^9 * .018 * 8410 = \$19{,}782{,}000$ Hence, the only unknown component of the revenues is the biofuel revenue (BR). The cost components are as operating costs (OC): $221,232,000.00/yr. Return on investment (ROI) depends on the total project investment (TPI) ($195,267,764), the discount rate (DR) (10%) and the equipment life span (ELS) (20 years).

$$ROI = \frac{DR * (1 + DR)^{ELS}}{(1 + DR)^{ELS} - 1} * TPI = \$?/yr \quad [37]$$

$$ROI = \frac{.1 * (1 + .1)^{20}}{(1 + .1)^{20} - 1} * 195{,}267{,}764 = \$20{,}713{,}857.58/yr$$

Income tax (IT) is calculated by the following equation by using federal income tax rate (TR), 35%.

$$IT = TR * (BR + ER - OC - DC) \quad [38]$$

$$IT = .35 * (BR + \$1{,}328{,}012 - \$221{,}232{,}000 - \$5{,}238{,}490)$$

where DC ($5,827,371/yr) is the depreciation cost of fixed investment by assuming a 20-year depreciation period for the process equipment

$$IT = .35BR - 78{,}799{,}867.3$$

Then, at the breakeven point, total costs should be equal to total revenues.

$$BR + ER = OC + ROI + IT \quad [39]$$

$$BR + 19{,}782{,}000 = 221{,}232{,}000 + 195{,}267{,}764 + .35BR - 78{,}799{,}867.3$$

$$.65BR = 317{,}288{,}967 ==> BR = \$489{,}121{,}379.5/yr$$

From the above calculation, the bioethanol revenue is $\$489{,}121{,}379.5$. The biorefinery plant simulation result shows that 182,263,202 kg per year of ethanol is produced. Ethanol density at ambient temperature is 0.789 g/cm^3. Using the that density at room temperature, the total volume of ethanol produced annually is 231,005,325.72877 liters per year. Using the above information,

$$MESP = \frac{Total\ Biofuel\ Revenue}{Total\ Ethanol\ Product\ Sale} = \frac{\$489{,}121{,}379.5}{231005325.72877\ \text{Liters/y}} = \frac{\$2.11735995}{Liter}$$

Therefore, the minimum ethanol selling price is estimated to be $2.1174/liter in Addis Ababa. When ethanol burns in combustion engine, it generates energy in the form of heat.

$$C_2H_5OH + 3O_2 == > 2CO_2 + 3H_2O + Heat$$

That heat energy is the holy grail of the plant and has a gasoline gallon equivalency (GGE) value of 1.5. This means that to replace the energy of 1 volume of gasoline, 1.5 times the volume of ethanol is needed. In this bioethanol process simulation, about 6,023894.722 mol of ethanol are produced annually. This means

$$1.5\frac{MBtu}{kmol} * 6023.894722\ kmol\ =\ 602.3895\frac{MBtu}{yr} = 6\frac{TBtu}{yr}$$

The overall amount of energy produced annually in the form of ethanol is about 6 TBtu. The plant simulation result indicated on the above estimation is comparable with the result of already installed biorefinery plants.

CHAPTER 6: **RESULT AND DISCUSSION**

The biorefinery plant was fully simulated. The energy and material balance were internally estimated using the software. Financial streams also calculated based on the input and result of the overall process. The cost for equipment, for erection, for operation and other overheads are estimated. The upstream process costs for feedstock, feedstock handling, pretreatment, enzymatic hydrolysis, co-fermentation, raw materials, equipment, construction, and other overheads. The downstream process covers the cost for product recovery, solid waste combustion, liquid waste treatment, ash disposal, marketing, and others. All the above cost was estimated and summed up in annual form. The operation produces a product, ethanol. Using the 2000 tonnes per day bagasse, the maximum hourly ethanol production was estimated to be 21672.16 kg/hr. Having that the annual ethanol production was also summed up to be 182,262,865,6 kg. This trend only shows the relationship between feed and product. However, the process was expected to change when the scale of the process varies. Irrespective of the geometrical variation, the feed rate is varied from 5000 kg to 100000 kg. Therefore, the relationship between the feed scaling up and ethanol production was also studied using sensitivity analysis as flow:

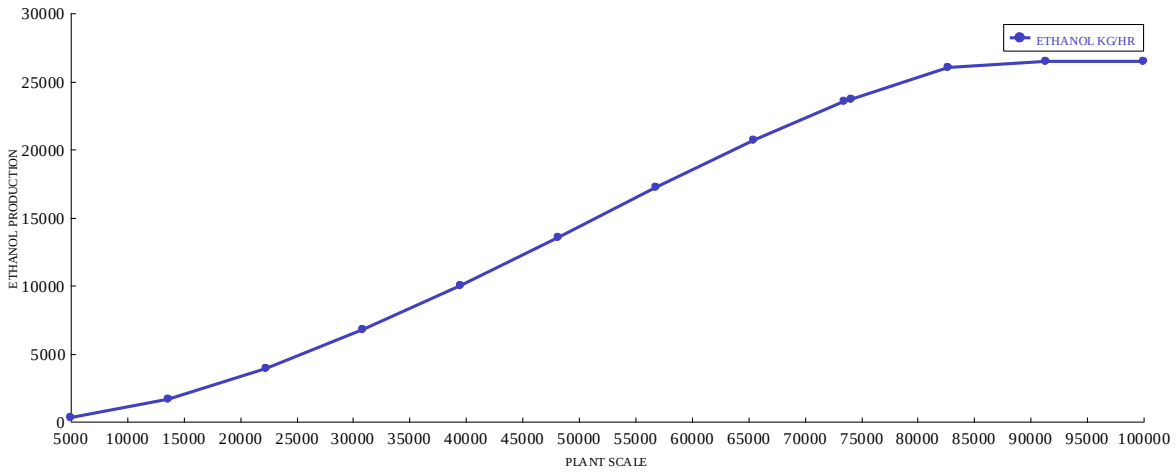


Figure 26 The relationship between plant scale vs ethanol production

The above graph clearly shows the relationship of increasing the feed rate with ethanol production. The relationship curve looks like as expected. However, from the point, 85000 kg/h to 100,000 kg/h, the ethanol production process changes its slope. This change may come from agitation challenge, dissolved oxygen challenge or any other transportation phenomena

Then, the main purpose of the plant is to generate a revenue by selling ethanol. The product, ethanol is assumed qualitatively to be competitive in local and global markets. As the simulation result indicates, the total annual revenue generated by selling ethanol at MESP is $489,121,379.5. The other revenue stream of the biorefinery plant is, excess energy. The excess energy is generated by burning solid waste of the plant and the excess is possible to sale to the national grid. According to the Activated Aspen Energy Analyzer, the total energy to saved is $1.1*10^9$ kcal/h. Then, by selling that energy in $0.018 kwh to national grid, about $19,782,000 additional revenue is generated. In general, the total gross revenue collected annually from the two revenue streams is estimated about $ 282,693,125.8538. The net profit is estimated by considering depreciation cost and federal 35% tax. When it is calculated before cutting the depreciation cost, the net profit is $203,532,531.8. if the depreciation cost is considered about $5,744,673.15 net profit is estimated. However, this is estimation is based on the calculated MESP and $0.018 excess electric selling price. Even though, the simulation result shows a positive value, the MESP, $2.1174/liter does not make it competitor on the local market with fossil fuel. Because the current average selling price of fossil fuel in Addis Ababa is about $0.72. So, the government should make some favor for the sake of the environmental protection and food vs fuel competition. If the government changes its renewable energy strategy and add some incentive and subsidy, the biorefinery plant will penetrate the market.

Table 14 Comparing simulation result with other already published in high impact journals

Parameters	**Design, 2019**	**NREL Report, 2012**	**Lili Zhao et.al., 2015**
MESP per Liter	$2.1174	$.7926	$1.417
MGSP per liter	$.72	$.75	$1.07
Profitability	Infeasible	Infeasible	Infeasible

6.1 SENSITIVITY ANALYSIS

Sensitivity of some factors is performed using Aspen Plus built-in function. The built-in function uses a single-point sensitivity analysis. So, the sensitivity analysis was performed on the Aspen model using the variables and limits. The result of sensitivity analysis has shown that feedstock cost, fermentation reaction and enzymatic hydrolysis had great impact

on ethanol production. Beyond that, the temperature for fermentation is the parameter selected for sensitivity analysis. This is because the mathematical model developed for enzyme kinetics had indicated as a greater impact on the fermentation process. As it indicated, the temperature affects the conversion process and determines the price of the ethanol.

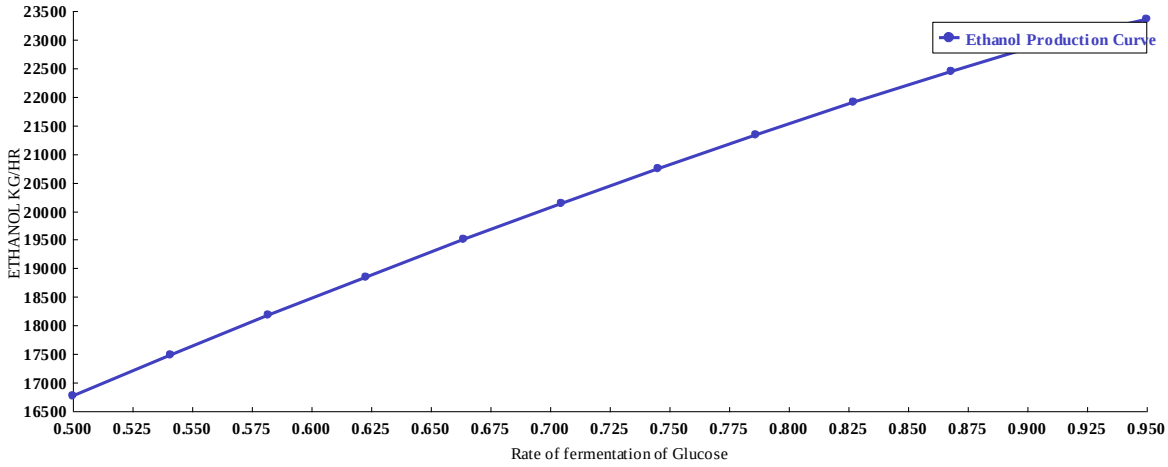


Figure 27 Sensitivity of Ethanol Production with respect to rate of fermentation of glucose

The above graph is a graph of percentage of glucose conversion vs ethanol production. The graph is uniform. It also shows that the conversion and ethanol production is positively related.

6.2 MARKET CONSIDERATION

The rigorous economic model including detailed estimates on investment cost, production cost and revenues streams. Because some additional cost related to ash disposal, purchase of sulfuric acid catalyst and fermentation nutrition is not considered at this point. In general, the local and global biofuel marketing share is increasing. For instance, Ethiopia's oil retail and distribution industry are a mature industry characterized by moderate growth rates, high barriers to entry, and engagement of few multinationals. There are about ten oil companies working in the country that could play crucial role in the blending of gasoline with ethanol and distribution of blended gasoline as well as other petroleum products. These companies are local, regional, and international, namely: Nile Petroleum, Libya Oil, NOC, TOTAL, Kobil, YBP, Daloal, WAS, TAF and Yetebaberut Beherawi Petroleum. The blending of gasoline and ethanol was given first to Nile Petroleum in 2008(Hiben 2013) as its facility was positioned well from the others in terms of place, capacity, and cost of upgrading to blending operation at Sululta, 26 km north of the capital, and now blending is shared by two

other blending companies including Nile Petroleum namely Oil Libya established in 2011 and National Oil Company (NOC) in 2012 at their facilities located in Addis Ababa and Dukem, 35 km south east of the capital. If everything goes as planned the current direction of TOTAL is also building its own blending station, forth for the country, that the company will start blending by itself (Abadi, 2013; Sherif, 2013; Tilahun, 2013). The price of feedstock in an international market seems declining. The decline seems steady from over $1500/ton in March, 2013 to $1000/ton in April, 2016, $45/ton and is expected to further decrease(Rodrigues Gurgel da Silva et al. 2018).

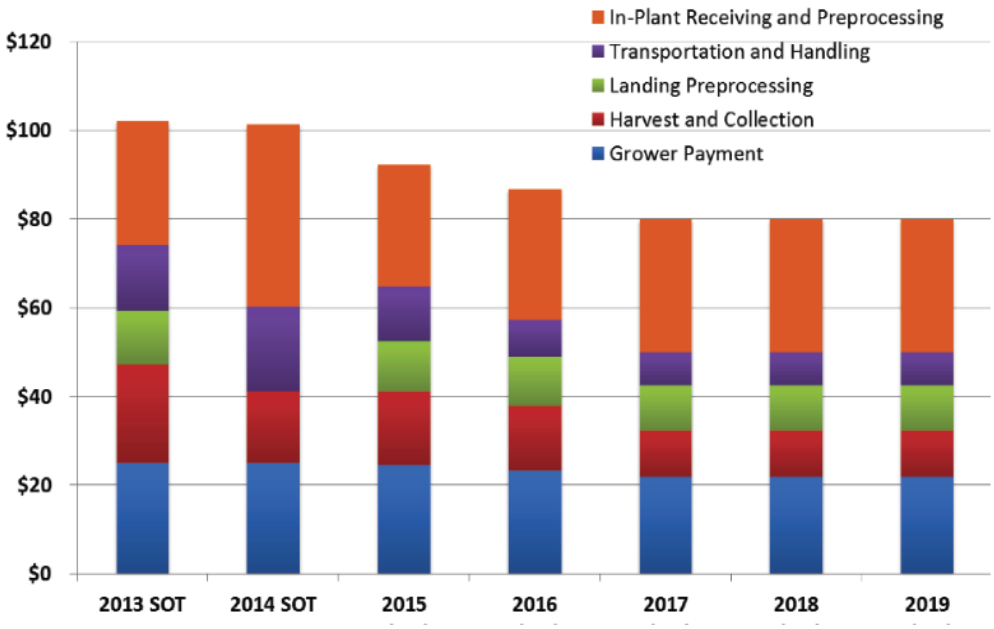


Figure 28 Global feedstock price declining trends

The same trend is observed for ethanol price too. Construction of such a plant would greatly influence the market price negatively, and it is uncertain if it would be economically feasible. However, the acid and enzymatic pretreatment process with subsequent washing allows for high adaptability. The prerequisite for such adaptability is appropriate sizing of the ethanol specific part of the plant, which would increase the initial investment costs.

All the three blending companies with the support of the steering committee established by the government from different organizations to evaluate and recommend the best blending option among the possible alternatives has agreed and built the facilities to employ the in-line blending mechanism. In the in-line blending system, gasoline and ethanol are blended in stream at the blender and a single finished product is loaded. The volumetric flow rate of gasoline and ethanol are pre-adjusted and automatically controlled depending on the fuel grade required. In this blending method, a precise blending level and a homogenous blend

can be attained through pressure mixing. The daily blending capacity of each company is said to reach up to 1500 m^3 of ethanol while the current daily consumption of ethanol and gasoline in the capital has been estimated at 24.5 m^3 and 368.5 m^3 respectively (Abadi, 2013; Sherif, 2013; Tilahun, 2013).

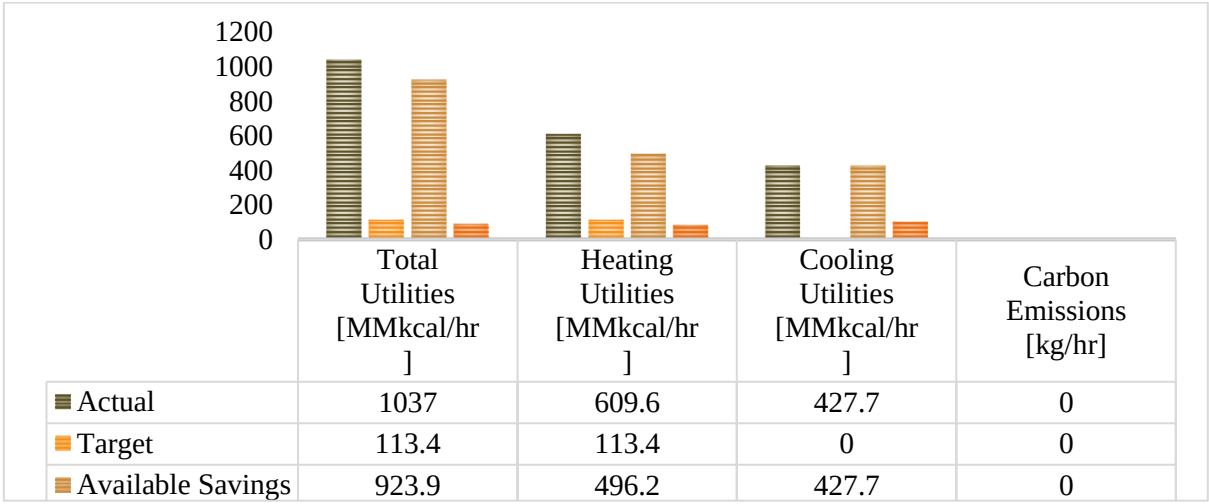
The import and distribution are entirely under the control of the government and prices are regulated often to avoid rapid changes. Currently, the marketing and distribution of blended gasoline as well as petroleum products is the responsibility of all the nine oil companies in accordance with the marketing and distribution agreement among the companies and the Ministry of Trade (MoT). The companies distribute the petroleum products imported either through the port of Djibouti or from facilities in Sudan and supplied to them by Ethiopian Petroleum Supply Enterprise (EPSE). Generally, as a joint business by different actors, Ministry of Trade is responsible to set prices of any fuel according to world market price and thus the contract with the ministry covers how the price correction will be done in cases of fluctuations. The contract with lignocellulosic and molasses bioethanol producers covers the quality criterion the bioethanol must fulfill and the delivery scheme.

6.3 CARBON AND ENERGY BALANCE

Biorefinery plant is a plant with almost natural process. The raw material-product conversion process is supported by microorganism with almost zero pollution. The emission from the plant is calculated according to 2007 carbon dioxide emission standard. However, there is possibility to emit carbon dioxide. The feedstock and the media for microorganism was added to the enzyme production, fermentation media. Those inlets can be source of carbon. Over 98% of the carbon enters as corn stover feedstock. Other carbon sources include corn steep liquor used as fermentation nutrition and cellulase enzyme for cellulose hydrolysis. The carbon balance is not fully closed, as carbon outlets totals to about 96% of total incoming carbon. Carbon in the form of CO_2 is accounted for in the flue gas stream. Carbon dioxide is produced from different location of the plant. One of the sources of the CO_2 for emission is fermentation and combustion modules. Most of the inlet carbon are converted into product as a form of ethanol. However, some are released as CO_2. The emission is through the flu gas treatment (scrubber).

6.4 ENERGY EVALUATION

The plant needs less amount of energy relative to other similar ethanol production processing techniques. This is because microorganism does the conversion. To run the plant, input energy is required in the form of steam and electricity. The biorefinery plant also generates solid waste. Instead of throwing the solid waste into landfill, some amount of energy is recovered through waste to energy technology. The main solid waste from the process is lignin. This is also a waste with high heating value. So, most of the heat for the plant is recovered from lignin through combustion technology. The amount of recovered heat is enough to run the plant. In addition to the heat recovered from lignin, some amount of energy in the form of biogas or methane is recovered from the anaerobic digester. Combining the two methods of heat recoveries, the plant becomes self-sufficient in energy. Not only being self-sufficient, but also generate another revenue stream by selling about 85% excess amount of energy, which is $19,782,000. The potential energy for material streams used in this analysis has three contributions:

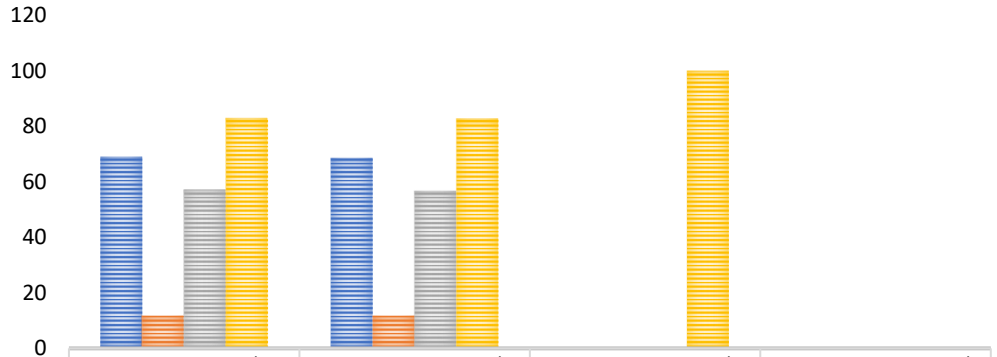


	Total Utilities [MMkcal/hr]	Heating Utilities [MMkcal/hr]	Cooling Utilities [MMkcal/hr]	Carbon Emissions [kg/hr]
Actual	1037	609.6	427.7	0
Target	113.4	113.4	0	0
Available Savings	923.9	496.2	427.7	0

Figure 29 Summary of Energy Flow from Aspen Energy Analyzer

Balancing the input and out energy needs some more considerations. The amount of carbon input and output carbon in different stages of the plant are incomparable. This is because, some biomass of microorganism are produces by eating them. This mean the mass of the biomass is the input carbon. The LHV is the energy released when a material is burned to form its combustion products, with water in the vapor phase. This is a true heating value for transportation fuels, where the combustion water is generally not condensed to recover heat. On an LHV basis, any liquid water present in a material stream therefore reduces its combustion potential because heat must be expended to vaporize that water. Note that the

sign convention in this basis follows the usual convention for heat of combustion: streams that can be burned (e.g., glucose or ethanol) have a negative potential energy. Streams that cannot be burned (e.g., water or sulfuric acid) have a positive potential energy.



	Total Utilities [$ Millions /Yr]	Heating Utilities [$ Millions /Yr]	Cooling Utilities [$ Millions /Yr]	Carbon Emissions [$ Millions /Yr]
Actual	69	68.5	0.5023	0
Target	11.76	11.76	0	0
Available Savings	57.24	56.74	0.5023	0
% of Actual	82.96	82.83	100	0

Figure 30 Summary of Energy Cost Generated from Aspen Plus V10

The energy losses from the cooling tower and combustion exhaust are large. Ambient heat losses are also significant; these include the wastewater lagoons and the air-cooled condenser on the rectification column.

6.5 SCENARIO ANALYSIS

In the case of Ethiopia, increasing price of imported petroleum has become a heavy burden and the use of bioethanol has been imagined to have positive implications mainly through substituting gasoline and facilitating improved energy security. However, the development of bioethanol could have long-term impacts together with the perceived benefits and hence undesirable consequences that may not be recognized at the early stage may introduce at a later stage if the right development track is not followed. This part, therefore, identifies the future shifts of extended bioethanol production and the possible scenarios towards contribution of ethanol as a transport fuel to discuss the key socio-economic and environmental benefits and difficulties in developing bioethanol sustainably so as benefit the country by taking protective measures at early stage to diminish the potential impacts at a later stage. With the fundamental changes to meet the growing energy demand there are many possible scenarios in the anticipated future. The key parameters for the developed

scenarios make happen will be the status of development in socio-economic benefits, environmental movement forces and security.

6.5.1 Ethanol Blending Scenarios

Blending biofuel with fossil fuel is a transitional stage for total shift. Blending is mixing two parts into one. So, adjusting the ration of mixing the two fuels whether the rate of shifting from biofuel to fossil fuel. There are three blending ratios taken as example for this scenario analysis.

Low Blend Scenario: The low blend scenario current alternating is 5% or 10% ethanol blend in Addis Ababa region is assumed to prolong with only 10% ethanol blend but still in the capital(Hiben 2013). As a result, 19.8 million liters of ethanol is required to satisfy the E10 target in Addis Ababa region in 2030 which is almost two-fold of the current production.

Medium Blend Scenario: In this scenario the use of ethanol will increase gradually rather than gasoline since it is assumed that the entire SI engine vehicles will use blended gasoline all over the country. Within the scope of this scenario, additional bioethanol quota of 5% was planned to be obligatory from the year 2015 in Addis Ababa region and then 15 % blend all over the country starting 2020 are considered as proposed by the government(Hiben 2013).

High Blend Scenario: This scenario assumes the national environmental and security movement. In this scenario though population, industrial output, passenger travel, and freight transport continue to rise, ambitious imported energy saving measures can allow doing more with locally available fuel. This is in striking contrast to business as usual projections, which predict ethanol demand will increase slightly. For high blending scenario, the proposal of 15% blend in the capital starting 2015, 20% blend all over the country starting 2020 and that of 25% starting 2025 are assumed to be accepted and enforced.

CHAPTER 7: **CONCLUSION & RECOMMENDATION**

7.1 CONCLUSION

After inserting all the necessary data for simulation, the economic profitability of the cellulose based biorefinery plant is techno-economically analyzed. The relationship between scaling up the feed rate and bioethanol production was found positive. In addition to that, the result of the simulation shows that the MESP is $2.1174 per liter. Currently the price of gasoline as referred online retailer in Addis Ababa shows that $.72 per liter. This number indicates that the price of fossil fuel per liter in Addis Ababa is cheaper than cellulosic bioethanol. Therefore, bioethanol based on lignocellulosic biomass is not able to compete with fossil gasoline in Ethiopia. Even in the most optimistic scenario with zero economic profit, the PGP of ethanol is $2.1174 per liter is higher in the current Ethiopia's pricing policy. However, if the key technical barriers that have major effect for ethanol production cost are removed by government, the development pathway is promising and has the potential to be profitable in Ethiopia.

7.2 RECOMMENDATION

It is obvious that lignocellulose based biorefinery plant is technically and economically proved as important to reduce environmental pollution and to settled down the fuel vs food computation. And, the simulation result showed us that such plant is incompetent with fossil fuel in Ethiopia market by the current energy market policy. However, the government can make lignocellulosic biomass based biorefinery plant competitive with fossil fuel. Few of the most recommendable measures that the government can take are feed-in tariff and compulsory purchase of electricity, direct subsidy, tax preference and finally R&D promotion.

1. Feed-in tariff and compulsory purchase of electricity: the biorefinery plant produces about $1*10^6$ kcal/hr excess electricity. To obtain byproduct credit, it is suggestable that the excess electricity produced by the ethanol plant be purchased compulsorily by the grid under a certain feed-in tariff program. So, Ethiopia government should reshuffle its energy policy to incorporate such motivational plants.
2. Direct subsidy. Subsidy is imperative, since the plant will suffer from financial loss even in the most optimistic scenario under Ethiopia's technical status. The minimum amount of subsidy is suggested to be exempting the tax (.35) and land rent.

3. R&D promotion: although this is not directly related with the biorefinery plant, excelling the science and engineering of biorefinery can reduce the production cost. So, strong support should be given to the R&D of the key technologies involved in lignocellulosic ethanol production, including technologies for five-carbon sugar ethanol conversion, and low-cost cellulase enzyme preparation, as they have a significant impact on the PGP of bioethanol.

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APPENDIX-1: LIST OF INPUT COMPONENTS

Table 15 List of Components used to simulate the biorefinery plant

Component	Property	Quantity	Units	Reference
H2O	-	-	-	Native Aspen component
ETHANOL	-	-	-	Native Aspen component
GLUCOSE	-	-	-	Native Aspen component (dextrose)
GALACTOS	-	-	-	Duplicate of GLUCOSE
MANNOSE	-	-	-	Duplicate of GLUCOSE
XYLOSE	DHFORM	-216752.65	cal/mol	Native Aspen component (d-xylose)
ARABINOS	-	-	-	Duplicate of XYLOSE
CELLOB	-	-	-	Cellobiose. Used native Aspen component sucrose
SUCROSE	-	-	-	Native Aspen component
GLUCOLIG	MW	162.1424		Glucose oligomers. Most properties from GLUCOSE;
	DHFORM	-192875.34	cal/mol	Back-calculated to match ΔHc of CELLULOS
GALAOLIG	-	-	-	Galactose oligomers. Duplicate of GLUCOLIG
MANOLIG	-	-	-	Mannose oligomers. Duplicate of GLUCOLIG
XYLOLIG	MW	132.11612		Xylose oligomers. Most properties from XYLOSE; MW is XYLOSE minus H2O
	DHFORM	-149412.58	cal/mol	Back-calculated to match ΔHc of XYLAN
ARABOLIG	-	-	-	Arabinose oligomers. Duplicate of XYLOLIG
EXTRACT	-	-	-	Organic extractives. Duplicate of GLUCOSE
LGNSOL	-	-	-	Solubilized lignin. Native Aspen component vanillin
HMF	MW	126.11		(5-hydroxymethylfurfural) Properties for HMF were estimated within Aspen using NIST TDE routines.
FURFURAL	-	-	-	Native Aspen component
AACID	-	-	-	Native Aspen component (acetic acid)
LACID	-	-	-	Native Aspen component (lactic acid)
XYLITOL	-	-	-	Native Aspen component
GLYCEROL	-	-	-	Native Aspen component
SUCCACID	-	-	-	Native Aspen component (Succinic acid)
NH3	-	-	-	Native Aspen component
H2SO4	-	-	-	Native Aspen component
NH4SO4	-	-	-	Native Aspen component (ammonium sulfate)
NH4ACET	PLXANT/1	-1.00E+20	atm	Native Aspen component (ammonium acetate) forced non-volatile
DAP	-	-	-	Native Aspen component (diammonium phosphate)

HNO3	-	-	-	Native Aspen component
NANO3	-	-	-	Native Aspen component
NAOH	-	-	-	Native Aspen component
CNUTR	-	-	-	Cellulase nutrient mix. Duplicate of glucose
WNUTR	-	-	-	WWT nutrient mix. Duplicate of glucose
DENAT	-	-	-	Denaturant. Native Aspen component (n-heptane)
OIL	-	-	-	Corn oil antifoam. Native Aspen component (oleic acid)
O2	-	-	-	Native Aspen component
N2	-	-	-	Native Aspen component
NO	-	-	-	Native Aspen component
NO2	-	-	-	Native Aspen component
CO	-	-	-	Native Aspen component
CO2	-	-	-	Native Aspen component
CH4	-	-	-	Native Aspen component
H2S	-	-	-	Native Aspen component
SO2	-	-	-	Native Aspen component
CELLULOS	DHSFRM	-233200.06	cal/mol	Native Aspen component with specified heat of formation; back-calculated
GALACTAN	-	-	-	Duplicate of CELLULOS
MANNAN	-	-	-	Duplicate of CELLULOS
XYLAN	Formula	C5H8O4 (monomer)		
ARABINAN	-	-	-	Duplicate of xylan
LIGNIN	-	-	-	Used native Aspen component vanillin (C8H8O3).
ACETATE	-	-	-	Used native Aspen component acetic acid
PROTEIN	Formula	CH1.57O0.31N0.29S0.007		Wheat gliadin

APPENDIX-2: COST INDEXES

Table 16 Chemical Engineering Plant and organic chemical Cost Index

Chemical Engineering Plant Cost Index for Equipment				Organic Chemistry Index for input chemicals			
Year	Index	Index	in Calcs	Year	US Producer Price Index	Calculated Index	Index Used
1991	361.3	372.4	361.3	1987	106.4	112.3	106.4
1992	358.2	374.6	358.2	1988	116.3	115.5	116.3
1993	359.2	376.8	359.2	1989	123.0	118.7	123.0
1994	368.1	379.1	368.1	1990	123.6	122.0	123.6
1995	381.1	381.3	381.1	1991	125.6	125.2	125.6
1996	381.7	383.6	381.7	1992	125.9	128.4	125.9
1997	386.5	385.8	386.5	1993	128.2	131.6	128.2
1998	389.5	388.1	389.5	1994	132.1	134.8	132.1
1999	390.6	390.3	390.6	1995	139.5	138.0	139.5

2000	394.1	392.5	394.1	1996	142.1	141.2	142.1
2001	394.3	394.8	394.3	1997	147.1	144.4	147.1
2002	395.6	397.0	395.6	1998	148.7	147.6	148.7
2003	402.0	399.3	402.0	1999	149.7	150.8	149.7
2004	444.2	401.5	444.2	2000	156.7	154.0	156.7
2005	468.2	403.8	468.2	2001	158.4	157.2	158.4
2006	499.6	406.0	499.6	2002	157.3	160.4	157.3
2007	525.4	408.2	525.4	2003	164.6	163.6	164.6
2008	575.4	410.5	575.4	2004	172.8	166.8	172.8
2009	521.9	412.7	521.9	2005	187.3	170.0	187.3
2010	550.8	415.0	550.8	2006	196.8	173.2	196.8
2011		417.2	481.7	2007	203.3	176.4	203.3
2012		419.5	483.9	2008	228.2	179.6	228.2
2013		421.7	486.1	2009	224.8	182.8	224.8
2014		423.9	488.4	2010		186.0	228.4
2015		426.2	490.6	2011		189.2	228.4

Source for input chemicals: SRI International Chemical Economics Handbook, Economic Environment of the Chemical Industry 2004 and for equipment: Chemical Engineering Plant Cost Index Magazine,

APPENDIX-3: MATLAB CODE FOR CO-FERMENTATION

```
function dc = zmobilis(t,c)

% dc(1) = mqg = c(1) = biomass growth rate based on glucose

% dc(2) = mqh = c(2) = biomass growth rate based on xylose

% dc(3) = mq = c(3) = biomass growth rate based on both glucose & xylose

% dc(4) = mg = c(4) = Glucose consumption rate

% dc(5) = mh = c(5) = xylose consumption rate

% dc(6) = metg = c(6) = ethanol production based on glucose

% dc(7) = meth = c(7) = ethanol production based on xylose

% dc(8) = met = c(8)= ethanol production based on both glucose and xylose

umaxG = 0.41; %maximum specific cell growth based on glucose

KSQG = .45; %Monon saturation constant substrate limitation constant for cell growth based on glucose

mTIQG = .289; %Threshold inhibitory ethanol concentration for cell growth based on glucose

mMQG = 5.72; %Maximum inhibitory ethanol concentration for cell growth based on glucose

KIQG = 3.8; % Substrate inhibition constant in cell growth from glucose
```

```
umaxH = .1; %maximum specific cell growth based on xylose

KSQH = 0.491; % substrate limitation constant for cell growth from xylose

mTIQH = .266; %Threshold inhibitory ethanol concentration for cell growth based on xylose

mMQH = 5.3; %Maximum Inhibitory Ethanol Concentration for cell growth based on xylose

KIQH = 6; %Substrate inhibition constants in cell growth based on xylose

zsmaxG = 1.9; %Maximum Specific Glucose utilization

KSSG = 3; %Substrate limitation constants for glucose utilization

mTISG = 6.32; %Threshold inhibitory ethanol concentration for glucose consumption

mMSG = 4.26; %Maximum inhibitory ethanol concentration for glucose consumption

KISG = 7.54; %Substrate inhibition constant in glucose consumption

zsmaxH = .27; %Maximum Specific Xylose utilization

KSSH = 0.3; %substrate limitation constant for xylose utilization

mTISH = .531; %Threshold inhibitory ethanol concentration for xylose consumption

mMSH = 8.12; %Maximum inhibitory for both consumption

KISH = 6; %Substrate inhibition constants in xylose consumption, 600 g/L

zetmaxG = 5.12; %Maximum Specific Ethanol Production based on glucose fermentation

KSETG = 6.32; %Substrate Limitation constant for glucose fermentation

mTIETG = 4.26; %Threshold inhibitory ethanol concentration for glucose fermentation

mMETG = 5.54; %Maximum inhibitory ethanol concentration for glucose fermentation

KIETG = 5.4; %Substrate inhibition constant in glucose fermentation,

zetmaxH = 8.9; %Maximum specific ethanol production based on xylose fermentation,

KSETH = 0.3; %Substrate limitation constant for xylose fermentation,

mTIETH = 5.31; %Threshold inhibitory ethanol concentration for xylose fermentation,

mMETH = .812; %Maximum inhibitory ethanol concentration for xylose fermentation,

KIETH = .6; %Substrate inhibition constant in xylose fermentation,

n = 0.01; %Weighting factor for glucose consumption, % Glucose Disappearance Rate

dc = zeros (8,1);

%Biomass Production from Glucose
```

```
dc(1)=umaxG*(c(1)/(KSQG+c(1)))*(1-(c(3)-mTIQG)/(mMQG-mTIQG))*(KIQG/(KIQG+c(1)));

%Biomass Production from xylose

dc(2)=umaxH*(c(5)/(KSQH+c(5)))*(1-(c(8)-mTIQH)/(mMQH-mTIQH))*(KIQH/(KIQH+c(5)));

%Total biomass production rate from using xylose and glucose

dc(3) = (n*dc(1)+ (1-n)*dc(2))*c(3);

%Glucose consumption rate

dc(4) = -n*zsmaxG*(c(4)/(KSSG+c(4)))*(1-(c(8)-mTISG)/(mMSG-mTISG))*(KISG/(KISG+c(4)));

%Xylose consumption Rate

dc(5) = -(1-n)*zsmaxH*(c(5)/(KSSH+c(5)))*(1-(c(8)-mTISH)/(mMSH-mTISH))*(KISH/(KSSH+c(5)));

% Ethanol from glucose production rate

dc(6) = zetmaxG*(c(4)/(KSETH+c(4)))*(1-(c(8)-mTIETG)/(mMETG-mTIETG))*(KIETG/(KIETG+c(3)));

% Ethanol from xylose production rate

dc(7) = zetmaxH*(c(5)/(KSETH+c(5)))*(1-(c(8)-mTIETH)/(mMETH-mTIETH))*(KIETH/(KIETH+c(5)));

% Total Ethanol Production Rate

dc(8) = (n*(dc(6) + (1-n)*dc(7)))*c(3);

end

% tspan = [0 24];

% c0 = [15:-2:1];

% ode45(@zmobilis, tspan, c0)

% legend ("biomass from glucose", "biomass from xylose", "biomass from

% both", "glucose consumption rate", "xylose consumption rate", "Ethanol from glucose production rate",
"ethanol from xylose production rate", "total ethanol production rate")
```

APPENDIX-4: MATLAB CODE FOR SACCHARIFICATION

```
% Define global variables

global k1r E1B E1TZ G K1ad K1IG Sc Sc2 G2 K2ad E2TZ E2max E1max Rs Rs2 G20 S0 K1IG2 K2IG X
K1IX k2r K2IG2 K2IX k3r K3M K3IG K3IX K1ad E1TZ E1max K2ad E2TZ E2max

% Define constants
```

```
K1ad=0.4; K2ad=0.1; E1max= 0.06; E2max=0.01; Ea= -5540;

S0 = input('Enter the Concentration of Cellulose between 0.1 and 500 (g/kg): ')

Amt_Cellulose = S0; G0=0.01; G20=0.01;

E1TZ=input('Enter the Enzyme concentration of exo and endo-glucanase between 0.01 and 1 (g/kg): ')

E2TZ=input('Enter the Enzyme concentration of Beta-glucosidase 0.01 and 1 (g/kg): ')

Tz=input('Enter the Temperature you would like this to happen between 30 and 55 degrees Celcius  ): ')

Sc=S0; G2=G20; G=G0;

% Substrate reactivity is an assumption based on figure 2

k1r45= 22.3; k2r45 =7.18; k3r45=285.5; K1IG2= 0.015;

K1IG=0.1; K1IX=0.1; K2IG2=132; K2IG=0.04;

K2IX=0.2; K3M=24.3; K3IG=3.9; K3IX=201;

X=0; R=1.987;

% Define the Arrhenius law and calculate the kinetic constants

k1r= k1r45*exp(-Ea/R*(1/(273 + 45) - 1/(273 + Tz)));

k2r= k2r45*exp(-Ea/R*(1/(273 + 45) - 1/(273 + Tz)));

k3r= k3r45*exp(-Ea/R*(1/(273 + 45) - 1/(273 + Tz)));

 % Dfine constraints

t_span = [0:0.1:1000];

 % Solve ODE for Cellulose

[t, product] =ode45('saccharification',tspan,[S0; G20; G0;]);

figure (1)

len_input = length(tspan);

%plot(t, product(1:len_input,1),'r',t, product(1:len_input,2),'g', t,product(1:len_input,3),'b');

semilogx(t,product(1:len_input,1),'r',t,product(1:len_input,2),'g', t,product(1:len_input,3),'b');

ylim([0 110]);

xlabel('Time (hours)');

ylabel('Amount of (g/kg)');

legend('Cellulose','Cellobiose','Glucose');
```