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Subject/Topic:

UTILIZATION OF COCONUT SHELL FOR BIOHYDROGEN GENERATION: SIMULATION- BASED STUDY

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DEDICATION

This work is dedicated to my parents, Mr. and Mrs. KARGBO and my friends who supported me throughout this journey.

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ABSTRACT

The growing need for renewable energy sources has driven attention of researchers in biohydrogen as a sustainable alternative to fossil fuels. This study explored the feasibility of producing biohydrogen from coconut shell waste in Sierra Leone through thermochemical gasification. Coconut shells, which constitute a significant portion of agricultural waste in the country, were characterized through proximate and ultimate analyses to determine their suitability as a feedstock. Aspen Plus was used for simulating the coconut shell biomass, and a dual fluidized-bed gasifier was modeled, incorporating kinetic parameters from validated literatures. The process simulated the decomposition, pyrolysis, oxidation, and reduction stages with steam as the gasifying agent. The sensitivity analysis was performed to assess the impact of key operating parameters, including temperature, pressure, and steam flow rate, on syngas composition.

The results showed that the model predicted mole fractions of Hydrogen 0.305 and Carbon monoxide 0.264, aligning closely with experimental values reported by (Yu et al., 2019) and (Agu et al., 2019), though Methane was underpredicted. The Root Mean Square Error values of 0.0449 and 0.0655 confirmed good model reliability and the sensitivity analysis revealed that increasing pressure decreased Hydrogen and Carbon monoxide while increasing Methane and Carbon dioxide, consistent with Le Chatelier's principle. Higher steam flow rates initially promoted Hydrogen formation but eventually diluted the syngas, lowering overall concentrations of Hydrogen, Carbon monoxide, and Methane. The temperature increased favored endothermic reactions, increasing Hydrogen and Carbon monoxide production while reducing Carbon dioxide and Methane yields.

The economic evaluation using Aspen Process Economic Analyzer demonstrated promising feasibility. The process required an estimated capital cost of USD 5.84 million and annual operating and raw material costs of USD 12.92 million and USD 10.9 million, respectively. The annual product sales projected USD 28.53 million, the payback period was 7.04 years, with a rate of return of 20%. These findings confirm that coconut shell gasification in Sierra Leone is both technically and economically viable, offering an environmentally friendly solution to waste management while contributing to renewable energy production.

KEY WORDS: Biohydrogen; Coconut shell; Gasification; Renewable energy; Economic analysis.

RÉSUMÉ

La demande croissante en sources d'énergie renouvelables a attiré l'attention sur l'hydrogène biologique comme alternative durable aux combustibles fossiles. Cette étude a exploré la faisabilité de produire de l'hydrogène biologique à partir de déchets de coques de noix de coco en Sierra Leone par gazéification thermochimique. Les coques de noix de coco, qui constituent une part importante des déchets agricoles du pays, ont été caractérisées par des analyses proximale et ultime afin de déterminer leur aptitude en tant que matière première. Le logiciel Aspen Plus a été utilisé pour simuler la biomasse de coque de noix de coco. Un gazéifieur à lit fluidisé double a été modélisé, intégrant des paramètres cinétiques issus de la littérature validée. Le procédé a simulé les étapes de décomposition, pyrolyse, oxydation et réduction, avec la vapeur comme agent gazéifiant. Une analyse de sensibilité a été réalisée pour évaluer l'impact de paramètres clés tels que la température, la pression et le débit de vapeur sur la composition du gaz de synthèse.

Les résultats ont montré que le modèle prédisait des fractions molaires d'hydrogène 0,305 et de monoxyde de carbone 0,264, en accord avec les valeurs expérimentales rapportées par (Yu et al., 2019) et (Agu et al., 2019), bien que le méthane ait été sous-estimé. Les valeurs de l'erreur quadratique moyenne 0,0449 et 0,0655 ont confirmé la fiabilité du modèle. L'analyse de sensibilité a révélé qu'une augmentation de la pression réduisait l'hydrogène et le monoxyde de carbone tout en augmentant le méthane et le dioxyde de carbone, conformément au principe de Le Chatelier. Des débits de vapeur plus élevés favorisaient initialement la formation d'hydrogène, mais diluaient ensuite le gaz de synthèse, réduisant les concentrations globales d'hydrogène, de monoxyde de carbone et de méthane. L'augmentation de la température favorisait les réactions endothermiques, augmentant la production d'hydrogène et de monoxyde de carbone, tout en réduisant les rendements de dioxyde de carbone et de méthane.

L'évaluation économique réalisée à l'aide de l'Aspen Process Economic Analyzer a démontré une faisabilité prometteuse. Le processus nécessitait un coût en capital estimé à 5,84 millions USD et des coûts annuels d'exploitation et de matières premières de 12,92 millions USD et 10,9 millions USD respectivement. Avec des ventes annuelles projetées à 28,53 millions USD, la période de retour sur investissement était de 7,04 ans, avec un taux de rentabilité de 20 %. Ces résultats confirment que la gazéification des coques de noix de coco en Sierra Leone est à la fois techniquement et économiquement viable, offrant une solution écologique à la gestion des déchets tout en contribuant à la production d'énergie renouvelable.

MOTS-CLÉS : Hydrogène biologique ; Coque de noix de coco ; Gazéification ; Énergie renouvelable ; Analyse économique.

ACRONYMS AND ABBREVIATIONS

APEA : Aspen Process Economic Analyzer

ASPEN : Advanced System for Process Engineering

ANN: Artificial Neural Network

BMFTR : German Federal Ministry of Research, Technology and Space

C: Carbon

CFD: Computational Fluid Dynamics

CO : Carbon Monoxide

CO_2 : Carbon Dioxide

CH_4 : Methane

Cl: Chlorine

FC: Fixed Carbon

FAO : Food and Agriculture Organization

H_2 : Hydrogen

H_2O : Water

IEA : International Energy Agency

IMP-EGH : International Master Programme in Energy and Green Hydrogen

LHV : Lower Heating Value

M : Moisture

MSW : Municipal Solid Waste

RMSE : Root Mean Square Error

UNEP : United Nations Environment Programme

VM: Volatile Matter

WASCAL : West African Science Service Center on Climate Change and Adapted Land Use

WHO : World Health Organization

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INTRODUCTION

BACKGROUND

The increasing demand for renewable energy can be attributed to two factors: the need to combat climate change and the requirement to bring the world to a halt in the use of limited fossil fuel sources (IEA, 2021). Bio-hydrogen is an excellent choice among renewable energies due to its capability to support the transition to renewable energy and could be applied on a wide scale such as transportation, electricity, and industry (Balat et al., 2009). Hydrogen is the lightest and most abundant element in the universe, so it is readily available for utilization in energy production (Turner, 2004). It possesses several desirable characteristics; it is colorless, odorless, very flammable, and clean, since its combustion yields water vapor and not greenhouse gases (Mazloomi, 2012). Importantly, hydrogen is an energy carrier and not an energy source and therefore must be produced from other materials prior to being utilized (Dincer et al., 2015). Today, most of the hydrogen produced are from fossil fuels using methods like steam methane reforming (SMR), which releases a significant amount of carbon dioxide (CO_2) and reduces its environmental benefits (Mazloomi et al., 2012). This means that there is need for sustainable ways to produce hydrogen like biological, thermochemical, and electrochemical processes using renewable biomass resources, especially to meet a low-carbon hydrogen economy (IEA, 2019; Kapdan et al., 2006).

Coconut (Cocos nucifera) is one of the most cultivated tropical crops that are of great agricultural, economic, and industrial importance, which is mostly found in humid coastal areas in Asia, Africa, and Latin America (Research Desk Consulting, 2023). Indonesia, the Philippines, and India are the major producers of coconut (Research Desk Consulting, 2023). These countries are the main source of the world largest coconut supply, with Indonesia producing about 17.19 million metric tons in 2022 (FAO, 2022). The countries where coconut are mostly grown for large scale production in Africa are Tanzania, Ghana, Nigeria, and Mozambique, and coconut production supports livelihood and food security (Muyengi et al., 2015). In Sierra Leone coconut production was 6.5 thousand metric tons of coconut in 2022, which is 3.14% higher than the previous years and its highest production ever (Helgi Library, 2023). It is estimated that the total waste of coconut is around 60–65% of the entire coconut mass (Obeng et al., 2020). Specifically, the coconut shell makes up about 15–20%, husk about 35%, and coir approximately 10–12% of the total weight of the fruit (Nath et al., 2022). Approximately 33.7–41.86% cellulose, 23.73–25.10% lignin, and 18.3–25.14% hemicellulose is found in shells (Devanesan et al., 2023); approximately 38.86% cellulose, 34.96% lignin, and 30% hemicellulose are found in husks (Ahmed et al., 2023); and approximately 45.84% cellulose, 43.44% lignin, and minimum hemicellulose are found in coir fibers (Rahman et al., 2023). These compositions allowed thermochemical and biochemical conversion technologies to produce valuable products like biochar, bio-oil, and bio-hydrogen (Devanesan et al., 2023; Kumar et al., 2019).

Coconut waste, such as shells, husks, and coir, contributes significantly to environmental degradation and global warming through burning and anaerobic decomposition in landfills, which release large quantities of carbon dioxide (CO_2) and methane (CH_4) into the atmosphere (Muriuki et al., 2024). When dumped in landfills, these wastes not only produce greenhouse gases but also occupy valuable space, causes leachate formation, and pose serious challenges to urban waste management (Parachute-Kalpavriksha, 2021). However, thermochemical conversion processes, specifically gasification, offer a sustainable solution to these environmental concerns. Gasification involves the partial oxidation of organic materials like coconut waste at high temperatures in a controlled oxygen environment, producing syngas a mixture of hydrogen, carbon monoxide, and methane that can be used for energy generation (Kumar et al., 2019). This process not only reduces the volume of coconut waste but also recovers energy from the byproducts, which can be utilized for electricity generation or as fuel in industrial applications (Umenweke et al., 2021). Bio-hydrogen produced from coconut shell through thermochemical processes can be used in various sectors, including transportation, power generation, and industrial applications, offering a cleaner alternative to conventional fossil fuels (Kumar et al., 2019). This can be a game-changer in the energy sector, where the demand for renewable energy solutions is growing.

PROBLEM STATEMENT

Coconut shell waste management in Sierra Leone has become a critical environmental issue that has so far received little attention. In 2022, the country produced approximately 6,500 metric tonnes of coconuts (FAO, 2023), yet the shells are largely discarded in open landfills or openly burned without structured recovery or recycling pathways (Kagbeni et al., 2025). This practice contributes significantly to methane emissions, harmful local air pollutants, and climate change impacts, particularly in densely populated cities such as Freetown, where municipal solid waste generation averages 742 tonnes per day, equivalent to 0.45 kg per person, with 53% of the stream composed of organic residues (World Bank, 2023; Kabba et al., 2025). Waste separation remains extremely limited, with only 4.2% of households practicing consistent sorting, while 65.2% never separate recyclables (Kagbeni et al., 2025; Mansaray Pearce, 2019). As a result, coconut shells, despite being a lignocellulosic biomass with strong potential for conversion, are underutilized and treated merely as waste rather than as a renewable resource. Globally, thermochemical gasification of lignocellulosic feedstocks has been identified as a promising pathway for producing biohydrogen, a clean and sustainable energy carrier that can reduce dependence on fossil fuels (Singh et al., 2021). In Sierra Leone, however, the technical and economic potential of utilizing coconut shell waste for biohydrogen production remains unexplored. To address this, the present study applies Aspen Plus modeling of a dual fluidized bed gasifier, using validated kinetic parameters to simulate decomposition, pyrolysis, oxidation, and reduction stages under varying operating conditions, combined with an economic assessment through the Aspen Process Economic Analyzer. This approach provides scientific evidence on the feasibility of coconut shell gasification as a waste to energy pathway, with the capacity to reduce landfill pressure, lower greenhouse gas emissions, improve urban air quality, create employment opportunities, and support Sierra Leone's transition toward clean energy and climate resilience.

RESEARCH QUESTIONS

I. What are the best operating conditions (temperature, pressure, gasifying agent) for maximizing biohydrogen yield from coconut shell?
II. How does the variation in input parameters affect the gasification process yield in terms of hydrogen?
III. What possible economic advantages can bio-hydrogen production bring through these feedstocks in Sierra Leone?

RESEARCH HYPOTHESES

The gasification of coconut shell waste is proposed as a transformative approach to simultaneously tackle the growing challenges of waste disposal and environmental degradation. It is expected that this process will yield biohydrogen and syngas, both of which offer promising alternatives to fossil fuels. Converting waste into valuable energy, this process holds potential to not only reduce carbon emissions but also accelerate the shift toward sustainable energy solutions, contributing to global climate change mitigation efforts.

RESEARCH OBJECTIVE

The main objective is to assess the feasibility of using coconut shell materials for sustainable bio-hydrogen production through gasification.

The specific objectives are:

I. Characterization and modelling the gasification process of coconut shells and identification of important operational parameter for the best possible biohydrogen yield.
II. Conduct Sensitivity Analysis on how variations in input parameters (temperature, gasifying agent, pressure) affect hydrogen yield.
III. To assess the economic benefits of bio-hydrogen production from coconut shell in Sierra Leone.

Chapter 1

LITERATURE REVIEW

1.1 BIOMASS

Biomass is any organic matter coming from plants or waste and potentially contains energy to produce electricity, heat, or fuels. These organic materials include carbon (C), oxygen (O), nitrogen (N), and hydrogen (H) that can be aquatic, like algae, or terrestrial, as in the case of wood, or solid waste, either urban and industrial or agricultural. Biomass is a part of the biodegradable fraction of these wastes that generates energy using thermal, chemical, or biochemical methods (Brás et al., 2012). Biomass is the carbon dioxide absorber from the atmosphere during photosynthesis and then releases the CO_2 back into the atmosphere after combustion. For this reason, biomass is neutral concerning CO_2 and is a sustainable and beneficial fuel that can replace fossil fuels as concerns about global warming increase (Tavares et al., 2020).

1.2 TYPES OF BIOMASSES

Biomass can be classified in two groups: waste and virgin biomass. These two groups can further be divided into 6 categories, as shown in Table 1.1

Table 1.1: Major groups of biomasses and their sub classification (Bhavanan et al., 2011).

Virgin	Terrestrial biomass	Forest biomass, grass, energy crops, cultivated crops
	Aquatic biomass	Algae, water plant
Waste	Municipal waste	Municipal solid waste biosolids, sewage, landfill
	Agricultural solid waste	Livestock and manures, agricultural crop residue
	Forestry residues	Bark, leaves, floor residues
	Industrial waste	Black liquor, demolition wood, waste oil or fat

The virgin biomass group includes production for energy. Representative species include eucalyptus, willows, poplars, assorghum, sugarcane, soya beans, sunflowers and cotton. The processing of these energy crops could take place via combustion, pyrolysis and gasification toward the production of biofuels, synthesis gas (syngas) and hydrogen (Bhavanan et al., 2011; Lasa et al., 2011).

With respect to waste biomass, farm waste is generated in enormous amounts. Among garden waste, rice husk is the most outstanding, accounting for 25% of rice weight. Other residues from plants are sugarcane fiber, coconut shell and husk, peanut shell, and straw. The examples in the farm waste category are animal manure such as cattle, chicken, and pork. Nevertheless, since the syngas with a low heating value are produced through the gasification of animal manure, this residue cannot be considered as a technical possibility for gasifier fuel. Yet this consideration may exist forest waste refers to another kind of biomass, and this may be used as a supplement to the mixing of animal manure; other waste biomasses are such as mill wood and tree and shrub wastes. Lastly, municipal and industrial waste are some other types of biomasses within the waste category such as Municipal Solid Waste (MSW), sewage sludge, and industry waste like black liquor from wood pulping. In addition to having rich raw material potential, they pose certain challenges during the gasification process, as they generate a large amount of ash deposits in the furnace or inside the boiler convective sections (Lasa et al, 2011).

1.3 BIOMASS CHARATERIZATION

1.3.1 Structure of Biomass

Biomass is a complex mixture of organic materials such as carbohydrates, fats, and proteins, along with small amounts of minerals such as sodium, phosphorus, calcium, and iron. The main components of plant biomass are extractives, fiber or cell wall components, and ash (Demirbaş, 2001).

Extractives: It includes substances present in vegetable or animal tissue that can be separated by successive treatment with solvents and recovered by evaporation of the solution. They include protein, oil, starch, and sugar (Rowell, 2012).

Cell wall: It provides structural strength to the plant, allowing it to stand tall above the ground without support. A typical cell wall is made of carbohydrates and lignin. Carbohydrates are mainly cellulose or hemicellulose fibers, which impart strength to the plant structure, while the lignin holds the fibers together. These constituents vary depending on plant type. Some plants, such as corn, soybeans, and potatoes, also store starch (another carbohydrate polymer) and fats as sources of energy mainly in seeds and roots (Rowell, 2012).

Ash: It is the inorganic component of the biomass (Demirbaş, 2001).

1.3.2 Components of Biomass

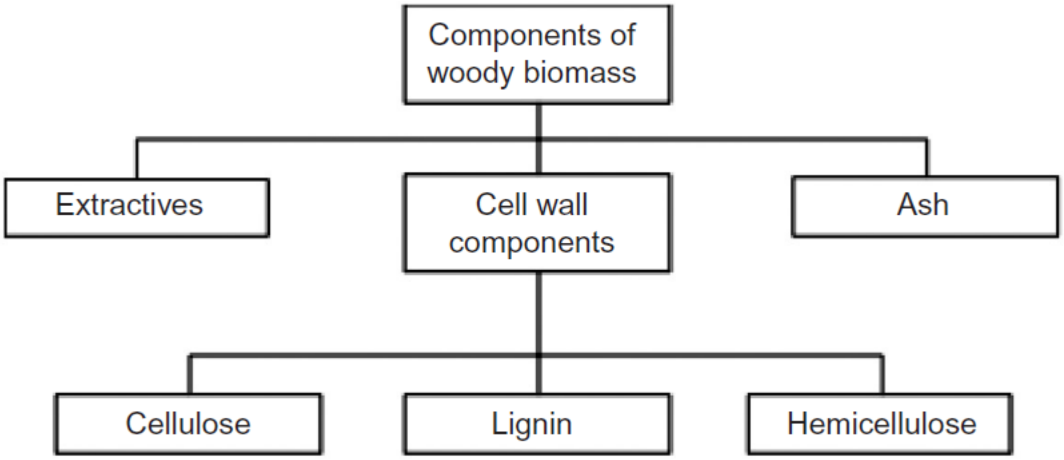


Figure 1.1: Major constituents of a woody biomass.

The main components of biomass include cellulose, hemicellulose and lignin. Cellulose is a glucose polymer and is a major constituent of the plant cell walls. Hemicellulose is a mixture of polysaccharides including glucose, xylose, galactose, mannose, arabinose and uranic acids, which can be linear or branched. Lignin can be considered as a high molecular weight amorphous group. It has the function of ensuring rigidity and resistance to the cell wall. Woody species are characterized by slow growth and are composed of tightly bound fibers, giving a hard surface, while herbaceous species have more loosely bound fibers, indicating a lower proportion of lignin. The ratio between cellulose and lignin is a determining factor in identifying the energy power of biomass. Since the biodegradability of cellulose is higher than that of lignin, biomass containing a higher proportion of cellulose to lignin provides a higher energy yield in processes that use biomass as raw material (Bhavanan et al., 2011; McKendry, 2002a). Table 1.2 shows some types of biomass and the respective typical percentages of cellulose, hemicellulose and lignin.

Table 1.2: Lignin, Cellulose and Hemicellulose content of different types of biomass (Bhavanan et al., 2011).

Plant	Lignin (wt. %)	Cellulose (wt. %)	Hemicellulose (wt. %)	Ash (wt. %)
Subabul wood	24.7	39.8	24.0	0.9
Wheat straw	16.4	30.5	28.9	11.2
Bagasse	18.3	41.3	22.6	2.9
Corn cob	16.6	40.3	28.7	2.8
Groundnut shell	30.2	35.7	18.7	5.9
Coconut shell	**28.7**	**36.3**	**25.1**	**0.7**
Millet husk	14.0	33.3	26.9	18.1

1.3.3 Composition of Biomass

Biomass consists of complex organic compounds such as, Moisture (M), and some amounts of inorganic impurities like ASH. Organic compounds contain four main elements: Carbon (C), Hydrogen (H), Oxygen (O), and Nitrogen (N). Biomass (e.g., Municipal Solid Waste and animal waste) may also have small amounts of chlorine (Cl) and sulfur (S). Biomass composition is important because it helps to design a biomass gasifier or a combustor. The two main types of composition analyses mostly used are the ultimate and proximate analysis methods (Basu, 2013).

- **Ultimate Analysis**

Except for moisture, M, and the inorganic components, ASH, the composition of the hydrocarbon fuel is represented in terms of its basic elements (Basu, 2013):

C + H + O + N + S + M + ASH = 100%

As we all know, not all biomass has these elements, most do not have sulfur (S). The fuel moisture content, or water content, is represented separately as M. Thus, only the hydrogen and oxygen found in the organic fuel components are considered hydrogen and oxygen in the final analysis rather than the hydrogen and oxygen found in moisture (Basu, 2013).

- **Proximate Analysis**

In proximate analysis, biomass is composed of its gross components, such as moisture (M), ash (ASH), volatile matter (VM) and fixed carbon (FC). Moisture was mentioned before, and it will be further explored here, as it is a very important characteristic of biomass. Some biomass can have up to 90% moisture, and because of this, much of the energy delivered in a gasification plant is for drying and evaporation, Proximate analysis can be expressed as (Basu, 2013).

FC + VM + M + ASH = 100%

Ash is the inorganic solid residue that remains after the fuel has burned all the way through. Its main components are silica, aluminum, iron, and calcium; it may also contain trace amounts of magnesium, titanium, sodium, and potassium. The ash obtained from biomass conversion does not necessarily come from the biomass itself. When collecting, biomass is generally scraped off the forest floor and then undergoes repeated handlings, during which it might pick up a large amount of dirt, stones, and other contaminants. These contaminants are frequently the largest inorganic portion of the biomass feedstock in many plants. Ash has usually a small contribution to biomass composition but may have a big impact on how biomass is used (Basu, 2013).

The condensable and non-condensable vapor that is emitted when a fuel is heated is referred to as its volatile matter. Both the rate of heating and the temperature to which it is heated affect how much there is (Basu, 2013). Fixed carbon is the solid carbon in the biomass that is still present in the char formed during the pyrolysis process after devolatilization. Char is not pure carbon and is not the fixed carbon of the biomass, while being a carbon residue after pyrolysis or devolatilization. It is referred to as pyrolytic char and, in addition to fixed carbon, also includes some volatiles and ash. Char from biomass is highly reactive and quite permeable (Basu, 2013).

FC is a crucial characteristic since, in most gasifiers, the pace of gasification and its yield are determined by the conversion of fixed carbon into gases. The size of the gasifier is decided using this conversion reaction, which is the slowest. Fixed carbon can be determined by (Basu, 2013):

$$FC = 1 - M - VM - ASH$$

1.4 PATHWAYS TO BIO HYDROGEN PRODUCTION

Hydrogen is also generally regarded as clean and high-energy fuel that releases only water when combusted and offers a highly promising prospect for decarbonization of energy systems (Show et al., 2011). Among all the various modes of production, bio-hydrogen; hydrogen produced from organic waste or biomass using biochemical or thermochemical processes provides an energy efficient and recyclable mode of production (Kapdan et al., 2006). The main techniques for bio-hydrogen production are usually categorized into biological and thermochemical routes, each comprising several distinct technologies with unique advantages and limitations (Hallenbeck et al., 2009).

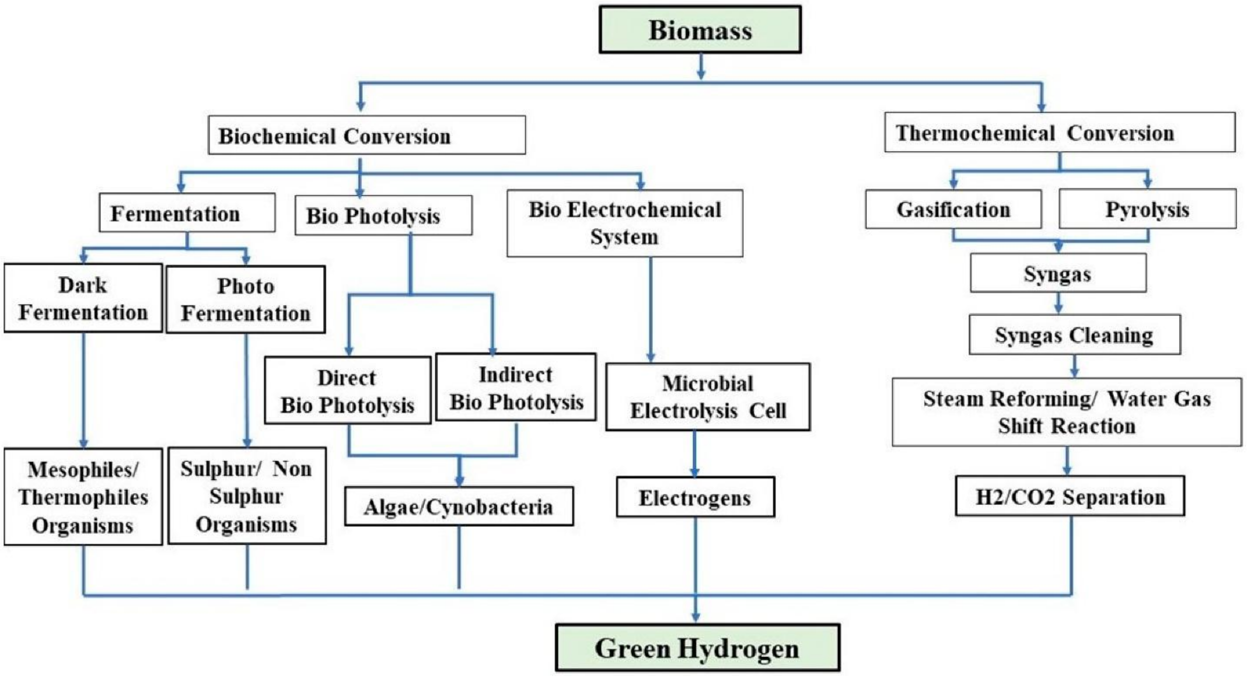


Figure 1.2: Various biohydrogen production pathways from biomass (Sharma et al., 2023)

1.4.1 BIOLOGICAL PATHWAYS

- **Dark Fermentation**

Dark fermentation refers to anaerobic dark reactions in which a variety of microorganisms, preferably species of Clostridium and Enterobacter, ferment substrates containing carbohydrates to produce carbon dioxide, hydrogen, and volatile fatty acids (Kapdan et al., 2006). This has been called "dark" because it typically uses hydrolysed biomass or single sugars as substrates and occurs in dark environments (Show et al., 2011). Although dark fermentation boasts the benefit of steady production of hydrogen and tolerance to a wide range of organic wastes, it is marred by low yields of hydrogen due to the formation of by-products such as acetate and butyrate (Hallenbeck et al., 2009). Moreover, the theoretical maximum yield is merely 4 moles of H_2 per mole of glucose under optimal conditions, even though actual yields are lower (Kapdan et al., 2006).

- **Photo-Fermentation**

Photo-fermentation uses photosynthetic purple non-sulfur bacteria, such as Rhodobacter sphaeroides, to ferment organic acids (acetate or butyrate) into hydrogen in the presence of light (Basak et al., 2007). This is catalyzed by nitrogenase enzymes, which are anaerobically active and utilize light energy for the transfer of electrons in hydrogen evolution (Basak et al., 2007). Photo-fermentation has the potential to provide greater hydrogen yields than dark fermentation, as it can recycle organic acids that are by-products of fermentation and thereby facilitate process integration (Show et al., 2011). However, its practical application is restricted by the requirement of constant light and low efficiency of conversion due to light intensity limitations and slow bacterial growth (Basak et al., 2007).

- **Biophotolysis**

Biophotolysis is a photochemical process wherein solar power is utilized to dissociate water into hydrogen and oxygen by cyanobacteria or green microalgae through photosynthetic processes (Hallenbeck et al., 2009). Biophotolysis can be divided into direct and indirect biophotolysis.

- **Direct Photolysis**:

It is a biological hydrogen production process in which light energy is directly used by photosynthetic microorganisms, cyanobacteria and green microalgae through special enzymes like hydrogenase or nitrogenase to split water molecules into oxygen and hydrogen (Scoma et al., 2012).

- **Indirect Photolysis**:

Is a biological process of hydrogen production in which photosynthetic microorganisms such as green algae and cyanobacteria undergo photosynthesis initially to produce and accumulate carbohydrates such as starch or glucose under aerobic conditions (Melis, 2002). The second stage then stored carbohydrates and break them down in the absence of oxygen (anaerobic conditions) to yield hydrogen gas by the activities of hydrogenase or nitrogenase enzymes (Ghirardi et al., 2000). This oxygen-hydrogen dichotomy of these two phases operates to protect oxygen-sensitive enzymes used to generate hydrogen (Hallenbeck et al., 2002). As a result, the process achieves higher yields of hydrogen compared to direct photolysis due to reduced enzyme deactivation by oxygen (Scoma et al., 2012).

- **Microbial Electrolysis Cells (MECS)**

Microbial electrolysis cells (MECs) are bio-electrochemical systems that use electrogenic bacteria to oxidize organic matter and generate an electric current, which is utilized to power hydrogen evolution at the cathode under applied voltage (Logan et al., 2008). MECs can utilize wastewater or effluents that are organic in nature as feedstocks and hence provide energy recovery and pollution abatement (Logan et al., 2008). But the disadvantages are that it needs external voltage supply, electrode material cost, and long-term operation stability (Show et al., 2011).

1.4.2 THERMOCHEMICAL PATHWAYS

- **Biomass Gasification**

Gasification is a thermochemical process in which biomass is converted into a combustible gas mixture (syngas) comprising hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2) by partial oxidation at high temperatures (700–1000°C) (Dong et al., 2016). This process is highly flexible, as it can handle a wide range of feedstocks including agricultural residues, forestry waste, and energy crops (Bridgwater, 2012). The syngas can be enriched in hydrogen by the water-gas shift reaction, where CO is reacted with steam to produce CO_2 and additional H_2 (Dong et al., 2016). Although gasification has high hydrogen production rates and industrial scalability, issues of tar formation, gas purification, and reactor design remain significant issues (Dong et al., 2016). This research work focuses more on the production of bio-hydrogen through biomass gasification.

- **Pyrolysis and Steam Reforming of Bio-Oil**

Pyrolysis is a thermal decomposition process carried out in an atmosphere of zero oxygen to obtain bio-oil, biochar, and syngas from biomass at temperatures of 400–600°C (Bridgwater, 2012). The resulting bio-oil can be subsequently steam reformed at high temperatures to yield hydrogen (Bridgwater, 2012). This two-step process allows for biomass conversion and hydrogen production to be conducted separately in terms of time and space, which yields logistical advantages (Dong et al., 2016). However, bio-oil will typically contain oxygenated compounds and impurities that will lead to catalyst fouling and require extensive pre-treatment or catalyst design (Bridgwater, 2012).

- **Supercritical Water Gasification (SCWG)**

Supercritical water gasification takes place at temperatures and pressures beyond the critical point of water (>374°C and >22 MPa), where water is a non-polar solvent and wet biomass is converted to gases without pre-drying (Kruse, 2008). SCWG can produce hydrogen-rich gas from algae, sludges, and wet biomass (Kruse, 2008). It gives maximum utilization of feedstock, reduced tar formation, and efficient conversion, according to Kruse (2008). However, the requirement for high-pressure reactors, corrosion-resistant systems, and control of salt precipitation presents serious technical as well as financial problems (Kruse, 2008).

1.5 GASIFICATION OF BIOMASS

Gasification is the conversation of solid or liquid biomass into useful and convenient gaseous fuel or chemicals by heating the biomass in a gasification medium such as oxygen (O_2), steam or air. These gases are composed of carbon monoxide (CO), hydrogen (H_2) and methane (CH_4). They can be burned to release energy or used for production of value-added chemicals (Mckendry, 2002b).

Both gasification and combustion are thermochemical processes, but they are different processes and there is an important difference between them. Whilst gasification is responsible for packing energy into chemical bonds in the product gas, combustion breaks those bonds to release energy. The gasification process adds hydrogen to and strips carbon away from the hydrocarbon feedstock to produce gases with a higher hydrogen-to-carbon (H/C) ratio, while combustion oxidizes the hydrogen and carbon into water and carbon dioxide, respectively (Kumar et al., 2010).

The process of biomass gasification involves reactions related to various phenomena such as drying (endothermic), pyrolysis (endothermic), oxidation (exothermic) and reduction (endothermic). In the drying phase, the moisture content of the biomass is reduced to less than 5%, occurring at temperatures of 100-200°C. In general, the moisture content of biomasses varies between 5-35wt.%. In the pyrolysis phase occurs the thermal decomposition of biomass, in the absence of oxygen or air, and volatile matter is released due to the thermal breakdown of biomass. As a result, gas mixtures containing oxygen, hydrogen, nitrogen and hydrocarbons are released, and the biomass is reduced to solid coal. Hydrocarbon gases condense at low temperatures and generate liquid tars. Gases released from the drying and pyrolysis zones may or may not pass through the oxidation zone, depending on the type of gasifier.

Combustion is a reaction between carbonized solid biomass and oxygen, resulting in the formation of CO_2. Hydrogen present in biomass is also oxidized to generate water (H_2O). The excessive heat released from carbon and hydrogen oxidation is used for drying, pyrolysis and gasification reactions. In gasification, various reduction reactions take place at temperatures ranging between 800 and 900°C. These reactions are mainly endothermic in nature (Patra et al., 2015; Molino et al, 2018).

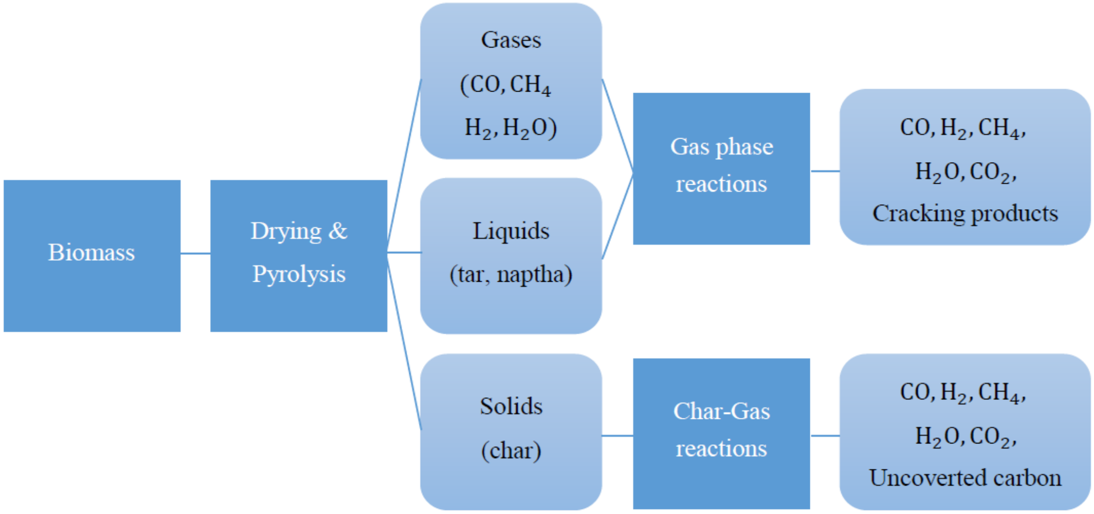


Figure 1.3: Reaction sequence of the gasification process (Kumar et al., 2019)

1.6 DESIGN OF GASIFIER

A gasifier is a reactor that converts carbonaceous material through chemical reactions. The two main type of gasifier are fixed bed and fluidized bed gasifier. There is a third type with a dragging suspension, but the feed needs to be finely divided, being infeasible for fibrous materials, such as wood, thus making the process unsuitable for most of the biomasses. Fixed bed gasifiers are divided into co-current and countercurrent bed and fluidized bed gasifiers between bubbling and circulating bed, as shown in Figure 1.4. Fixed bed reactors are mainly used for small scale production. On the other hand, in the fluidized bed reactors, bubbling bed reactors are recommended for medium scale production and circulating bed reactors for industrial scale processes. These 4 variations represent over 95% of the gasifier configurations, with less than 5% intended for variants of the two main models (Maniatis, 2001; McKendry, 2002c; Molino et al, 2016).

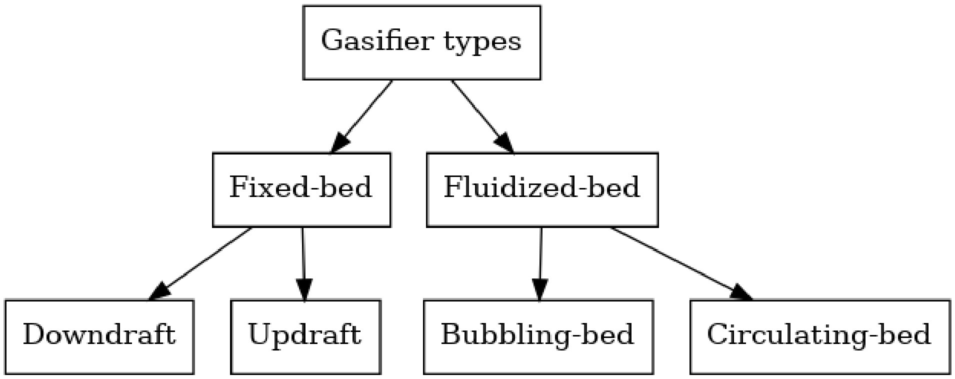


Figure 1.4: Main gasifier types (Panwar et al., 2012).

- **Fixed-Bed Gasifiers**

Fixed-bed gasifiers are the most common gasifiers for producing syngas. This type of gasifiers is easy to build and operate. Besides, Fixed-bed gasifiers can also be built in a small size. With these advantages, they are widely used in industry. They can be classified into two, Updraft gasifier and Downdraft gasifier.

Updraft gasifier, in this reactor, fuel is fed from the top and moves downward through the drying, pyrolysis, reduction and the combustion zone. While the gasifying agent is fed from the bottom and moves upward. Figure 1.5 shows an updraft gasifier. High cold-gas efficiency is an advantage of the updraft gasifier (Basu, 2013).

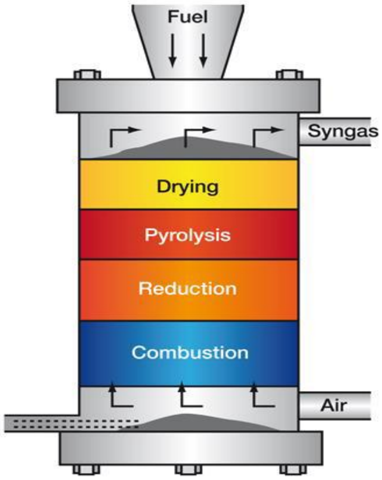


Figure 1.5: Updraft gasifier (Puig-Arnavat, 2011)

Downdraft gasifier, gasifying agent is fed at a certain height below the top as it is shown in Figure 1.6. The fuel is fed at the top through the drying, pyrolysis, combustion and reduction zones. The product gas then flows out from the lower zone. Compared with the updraft gasifier, it has a lower tar production rate (Basu, 2013).

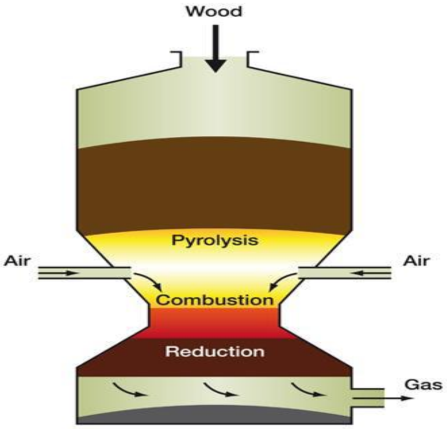


Figure 1.6: Downdraft gasifier (Puig-Arnavat, 2011).

- **Fluidized-Bed Gasifiers**

Fluidized bed gasifiers have been executed for coal gasification. Compared with the fixed bed gasifier, the greater uniform temperature distribution in the gasification zone is achieved by using bed material to cause the fluid and solid mixture to behave as a fluid under certain conditions. The fluidized-bed gasifiers can be classified into two main types: bubbling fluidized-bed gasifiers and circulating fluidized-bed gasifiers (Basu, 2013).

Bubbling fluidized-bed gasifier, air is fed at the bottom through the grid. Above the grid, the fuel is introduced into the vessel while the bed material is fed at the opposite side of the wall. The product gas goes into a cyclone where the solid particle is separated. Figure 1.7 shows a schematic of a bubbling fluidized-bed gasifier.

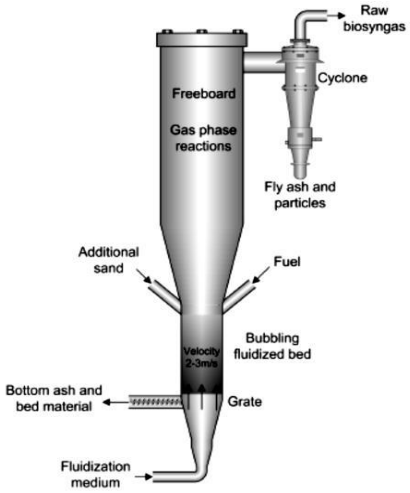


Figure 1.7: Bubbling fluidized-bed gasifier (Puig-Arnavat, 2011).

Circulating fluidized-bed (CFB) gasifier is composed of a vessel called riser, a cyclone and a solid recycling device. Figure 1.8 shows a schematic of a circulating fluidized-bed gasifier. Unlike the bubbling fluidized-bed gasifier, the separated bed material is recycled into the riser, thus a circulation of the bed material between the riser and the cyclone. In a circulating fluidized-bed gasifier, the fluidization velocity is higher than the velocity in the bubbling fluidized-bed gasifier. There are many commercial applications based on the circulating fluidized-bed technology (Basu, 2013).

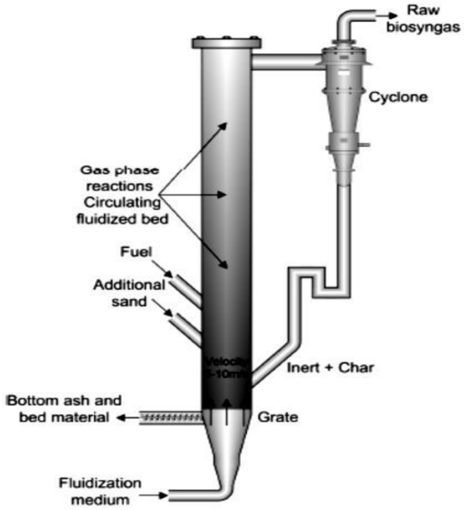


Figure 1.8: Circulating fluidized-bed gasifier (Puig-Arnavat, 2011).

1.7 ASPEN PLUS INTRODUCTION

Aspen Plus is a market-leading input software with a problem-oriented approach that can be used to more easily calculate physical, chemical, and biological processes. Which is widely used by world's leading chemistry organizations and related industries. It is a joint project called Advanced System for Process Engineering (ASPEN) started by Massachusetts Institute of Technology (MIT) and the US Department of Energy In the 1970's and finished in 1981. AspenTech was founded in the same year, and the ASPEN project was commercialized by AspenTech called Aspen Plus (Sun, 2012).

Aspen Plus is used in the industrial chemical process modeling, simulation, optimization, sensitivity analysis and economic evaluation. It provides comprehensive physical property models and the library of unit operation models, fast and reliable process simulation functions, and advanced calculation methods. With the physical property database and the operation models provided by Aspen Plus, engineers can simulate actual plant behavior effectively and accurately, thereby improving productivity and reducing the costs (Aspen Technology, Inc., n.d).

1.8 GASIFIER SIMULATION MODELS

Commercial plants require optimal operating parameters to achieve maximum interest. The operating parameters are often obtained by conducting experiments on pilot plants. The processes and equipment operate following the sequence of input data, data processing and return output data. This data is mass flows, temperatures, compositions and pressures. Although accurate data can be obtained through the experiments, it is always expensive and takes a lot of time to get the results. If these actions are done without prior study, the experimental data obtained may not be satisfactory and time and money have been spent on incorrect reactor sizing and operation (Li et al, 2001; Abdelouahed et al., 2012).

Modeling or simulation of a plant may not predict the process very accurately, but a good simulation model can help the engineers find out the effects of changing different parameters on the process results thereby optimizing the operating conditions efficiently (Basu, 2013). Modeling and simulation of gasification systems help in predicting the outlet gas composition when operating conditions and scale size change. This assists in planning the construction or retrofitting of existing equipment. The set of chemical reactions, fluid dynamics, and heat and mass transfer phenomena involved in this process make modeling a complex task (Li et al., 2001)

Gasifier simulation models can be classified into four groups (Basu, 2013; Ahmed et al., 2012), they are:

- Thermodynamic equilibrium
- Kinetic Modelling
- Computational fluid dynamics (CFD)
- Artificial neural network (ANN)

In Aspen Plus, thermodynamic equilibrium and kinetic models are often used to simulate the gasification process.

- **Thermodynamic Equilibrium Models**

The basic principle of using thermodynamic equilibrium models is the equilibrium state gives the maximum conversion under certain conditions. In these models, the reactions are zero-dimensional, and they are independent with time. The reaction kinetics and the reactor hydrodynamics are not considered in the thermodynamic equilibrium models. There are two types of equilibrium models: stoichiometric and non-stoichiometric. The stoichiometric model is based on equilibrium constants, which may limit the study since such constants are restricted to certain temperature and pressure conditions and are not always easily found for all reactions (Rodrigues, 2015).

Nonstoichiometric method, the reacting system has minimum Gibbs free energy when the equilibrium is reached. This method is also called Minimization of the Gibbs free energy method. The advantage of this method is that there is no need for the establishment of a specific set of reactions to solve the problem, requiring knowledge of only proximate and ultimate analysis. It is a simple model and can be used when the molecular formula is not known. Therefore, the nonstoichiometric method is suitable for biomass gasification simulation as the exact chemical formula of biomass is unknown and the gasification reaction mechanisms are very complicated (Carvalho, 2012; Rodrigues, 2015; Sun, 2014).

- **Kinetic Modelling**

Kinetic models make use of the detailed mechanisms of the chemical reactions involved, considering reaction rates, residence time, and hydrodynamics (Li et al., 2004; Buragohain et al., 2010). These are terms that introduce realism to this model and can be used to describe processes at any point and time in the reactor (Li et al., 2004; Buragohain et al., 2010). All these parameters, however, complicate the modeling process due to the number of simultaneous and parallel reactions assumed (Li et al., 2004; Buragohain et al., 2010). The amount of data required may discourage the use of this type of model, as the accuracy of the data used directly influences the quality of the resulting predictions (Li et al., 2004; Buragohain et al., 2010).

1.9 APPLICATION OF HYDROGEN

Hydrogen is increasingly recognized as a versatile energy carrier capable of decarbonizing various industries, including transport industry, and electricity generation (Dincer et al., 2015). Hydrogen fuel cells for transportation offer a clean alternative to fossil fuels, with good energy efficiency and no tailpipe emissions (Zhao et al., 2021). Hydrogen can be used for long-term energy storage to enable the integration of renewable energy sources like wind and sun into the electric power grid (Staffell et al., 2019). Hydrogen is important in various industrial processes in industry such as the production of ammonia, petroleum refining, and synthesis of methanol (Ball et al., 2015). Emerging uses of hydrogen include its application as a reducing agent in steel production to replace carbon-dense coke (Hyundai Steel, 2020). The ability of hydrogen to be liquefied and transported makes it a great option for international energy trade, especially between renewable-rich and energy-scarce regions (IEA, 2019). Hydrogen can be blended in the domestic market with natural gas or used directly in fuel cells to provide clean heat (Dodds et al., 2013). Hydrogen backup power systems provide safe electricity during power disruptions, particularly in critical buildings like hospitals and data centers (Ruth et al., 2020). Its use in synthetic fuel production also helps the shipping and aircraft industries reduce carbon emissions (Parra et al., 2019). The multi-sector flexibilities of hydrogen make it a cornerstone of net-zero energy systems (Bicer et al., 2017).

Chapter 2

MATERIALS AND METHODS

2.1 STUDY AREA

Sierra Leone, a West African country situated between latitudes 7° and 10° N and longitudes 10° and 13° W. Sierra Leone shares borders with Guinea to the northeast, Liberia to the southeast, and the Atlantic Ocean to the west. The country has a total land area of approximately 71,740 square kilometers and an estimated population of 8.4 million people, with the majority residing in rural areas (World Bank, 2024).

This research work is focused on Utilization of coconut shell waste from Sierra Leone where coconut cultivation occurs more in the riverine districts and coastal regions. Some of the key coconut-producing districts include Western Area urban district, Port Loko district, Kambia district, Bonthe district, Pujehun district and Moyamba district. Coconuts are produced in these areas for household consumption, small-scale processing of coconut oil, and market sales. Due to inadequate waste management facilities, coconut shells are often disposed of in the wrong way, resulting in environmental pollution by open burning and landfilling (UNEP, 2021).

2.2 SAMPLE PREPARATION AND PRE-TREATMENT

The coconut shell sample was collected from the Lomé market and prepared at the WASCAL laboratory at the University of Lomé, where it was initially ground and measured to a weight of 287.4 g. The sample was then oven-dried for 24 hours and stored in a bottle for two weeks before being transported to Germany. Upon arrival at the University of Rostock, the sample was taken for proximate and ultimate analysis. The final analyses were carried out at the Technical Laboratory of Waste Management and Bioenergy, Department of Waste and Resource Management, Faculty of Agriculture, Engineering and Environmental Science, University of Rostock

2.3 FEEDSTOCK CHARACTERIZATION

The selected biomass source for this study is coconut shell. Experimental analysis was conducted to determine both the proximate and ultimate properties of the biomass. The sulfur content was obtained from the ultimate analysis , while Table 2.1 presents the biomass feedstock and steam feed data. This study mass flow rate for the coconut shell is 7000Kg/h which was assumed to be used in the Aspen Plus simulation to know the amount of hydrogen produced.

- **Proximate Analysis**

To determine the proximate analysis of coconut shell, the analyses were conducted using standardized method with a LECO TGA701 Thermogravimetric Analyzer. The moisture content, volatile matter, ash content, and fixed carbon were all analyzed in the lab, and the results of the experiments as well as the analysis procedures were given for this study. The moisture content and volatile matter were determined using the TGA701 under program-controlled thermal programs, during which mass loss because of evaporation of water and loss of the volatile content was monitored. Ash content was determined according to DIN EN ISO 21656 (2021-06) Verfahren A, by the exposure of the biomass sample at elevated temperatures in an oxygen-rich atmosphere until complete organic combustion was attained. Fixed carbon was measured by difference of total sample weight minus the sum of moisture content, volatile matter, and ash content. The proximate analysis values were utilized as important input parameters for the modeling and simulation of coconut shell gasification using ASPEN PLUS.

- **Ultimate Analysis**

To determine the elemental composition of the coconut shell, an ultimate analysis was conducted using standardized methods. The standard procedure DIN EN ISO 21663 (2021-03) for solid biofuels elemental analysis was followed in the analysis of carbon, hydrogen, and nitrogen composition. The sulfur content was calculated according to DIN EN 15408 (2011-05), whereas ash content was calculated according to DIN EN ISO 21656 (2021-06). Elemental balance was used to calculate chlorine. The oxygen content was calculated by subtracting the determined elemental percentage according to DIN 51733 (2016-04) from 100%. The above analyses were applied to form the input parameters required for the modelling and simulation of coconut shell gasification in ASPEN PLUS.

Table 2.1: Specification of biomass and Steam feed

Stream	Component	Temperature	Pressure	Mass flow rate	Source
BIOMASS	Specified as its ultimate, proximate and sulfur analysis	800°C	1 atm	7000 kg/h	This Study
STEAM	H_2O	450°C	1 atm	Steam to biomass ratio (S/B) is 0.6	Doherty et al., 2013

2.4 COMPONENTS

All the components were properly defined before the simulation started. The simulated components of the simulation are defined in table 2.2. They were considered nonconventional solid components due to uncertainty about the precise formulas for biomass and ash. Enthalpy and density were only calculated during the simulation for these components. The coal-derived products, Aspen Plus has special models that may be utilized to calculate density and enthalpy. The biomass can be thought of as material derived from coal, such models can also be used to estimate the properties of biomass.

Table 2.2: Detailed data of the components modeled in the simulation.

Component ID	Type	Component name	Formula
BIOMASS	Nonconventional	-	-
ASH	Nonconventional	-	-
C	Solid	CARBON-GRAPHITE	C
WATER	Conventional	WATER	H_2O
S	Conventional	SULFUR	S

CO	Conventional	CARBON-MONOXIDE	CO
CO_2	Conventional	CARBON-DIOXIDE	CO_2
N_2	Conventional	NITROGEN	N_2
O_2	Conventional	OXYGEN	O_2
METHANE	Conventional	METHANE	CH_4
H_2	Conventional	HYDROGEN	H_2
CL_2	Conventional	CHLORINE	CL_2

2.5 PHYSICAL PROPERTIES

The PENG-ROB property method was used for this simulation, applying the Peng-Robinson equation of state to handle nonpolar and mild polar mixtures. The MIXCINC stream class was chosen to model the incompressible, solid-like behavior of the ground coconut shell biomass. A kinetic model was incorporated to simulate time-dependent chemical reactions during biomass conversion. This combination ensured accurate representation of both thermodynamic and reaction behaviors in the process.

Since biomass and ash were defined as nonconventional components, only the density and enthalpy were calculated during the simulation. HCOALGEN was selected as the enthalpy model for both biomass and ash, the density model was DCOALIGT. Different empirical correlations for heat of combustion, heat of formation and heat capacity are included in the HCOALGEN model.

2.6 KINETICS PARAMETERS

In this study, a kinetic modeling approach was used to simulate the gasification process. Unlike thermodynamic models that predict equilibrium composition based solely on energy minimization, kinetic models are dynamic and provide detailed insight into how fast individual reactions occur under varying operating conditions.

The chemical reactions in the gasification process were represented using an Arrhenius-based rate equation, where the reaction rate depends on temperature, gas concentration, and reaction-specific parameters: the pre-exponential factor (A), activation energy (E), and reaction order exponents. These parameters were obtained from validated literature sources and reflect experimental or semi-empirical data relevant to gas-solid and gas-phase reactions in biomass and hydrocarbon gasification systems.

In total, seven reactions were considered in the kinetic model, including partial and complete oxidation of carbon, steam-carbon reaction, the water-gas shift and reverse water-gas shift reactions, the Boudouard reaction, and methane steam reforming. The inclusion of these reactions enables a more accurate and comprehensive prediction of syngas composition, carbon conversion efficiency, and overall reactor performance. Tables 2.3 and 2.4 present the gasification reactions and their respective kinetic parameters used in this simulation.

Table 2.3: The gasification reactions for this simulation process (Masmoudi, et al., 2017)

Gasification Reactions	Reaction	Type of Reaction
Partial Oxidation	$2C + O_2 \rightarrow 2CO$	Exothermic
Complete Oxidation	$C + O_2 \rightarrow CO_2$	Exothermic
H_2O Gasification	$C + H_2O \rightarrow CO + H_2$	Endothermic
Forward Water-Gas Shift Reaction (FWGS)	$CO + H_2O \rightarrow CO_2 + H_2$	Exothermic
Boudouard	$C + CO_2 \rightarrow 2CO$	Endothermic
Reverse Water-Gas Shift Reaction	$CO_2 + H_2 \rightarrow CO + H_2O$	Endothermic
Methane Steam Reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$	Endothermic

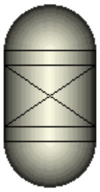
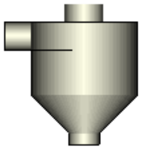
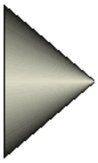
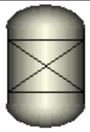
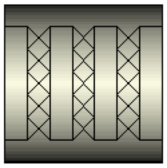
Table 2.4: Reaction kinetics for this model (Masmoudi, et al., 2017)

Reactions	A	E [J/kmol]	constants of exponents	
R1	1.47e+5	1.13e+8	-	1
R2	5.67e+9	1.6e+8		1
R3	8.268	1.882e+8	-	1
R4	2.78	1.26e+7	1	1
R5	8.268	1.882e+8	-	1
R6	1.785e+12	3.26e+8	1	0.5
R7	3.015e+6	1.2552e+8	1	1

2.7 BLOCKS SPECIFICATION

After specifying the inlet streams, all the blocks were specified according to the design operating condition. Table 2.5 gives a brief description of the unit operation blocks presented in the flowsheet. Table 2.6 gives detailed operating parameters for the blocks.

Table 2.5: Description of the blocks used in the modeling

BLOCK NAME	SCHEME	BLOCK ID	DESCRIPTION
RYIELD		DECOM	Breaks nonconventional biomass into conventional components and transforms biomass into carbon, ash and volatiles
RGIBBS		PYRO	Convert volatiles fragments into gases, liquid or char
SPLITTER		SPLITTER	Separates pyrolysis gases and solid char
MIXER		MIXER	Mix gases with injected steam for reforming
SEPERATOR		SEP1, SEP2	SEP1: Solid–gas separation (char removal) SEP2: Final gas separation (e.g., H_2 purification)
RPLUG		OXI, RED	OXI: Oxidation zone (char partial oxidation) RED: Reduction zone (gas-solid reactions)

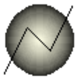
EXCHANGER		COOLER	Heat exchanger to cool syngas before final separation

Table 2.6: Operating parameters for the blocks

Block ID	**Temperature (°C)**	**Pressure (atm)**	**Specification**
DECOM (RYIELD)	800	1	Biomass decomposed into elemental pseudo components. Yields defined via RYield calculator block
PYRO (RGIBBS)	800	1	RGibbs used to simulate volatile product formation under equilibrium conditions. All species treated as products
SPLITTER	800	1	Volatile gas is separated from solid carbon/ash. Split defined manually or by design spec
MIXER	800 (Gas) / 450 (Steam)	1	Steam and gas-phase products mixed before entering oxidation zone
OXI (RPLUG)	800	1	Simulates partial oxidation. Kinetics can be added.
RED (RPLUG)	800	1	Reduction zone where reactions such as Boudouard and water-gas shift occur. Plug flow model.
COOLER (EXCHANGER)	700 → 25	6	Reduces syngas temperature from 700°C to 25°C before separation.

SEP1 (SEPARATOR)	800	1	Solid–gas separation; removes char from gas stream.
SEP2 (SEPARATOR)	25	1	Hydrogen purification and gas separation; pressure swing or membrane simulated.

2.8 CALCULATOR SPECIFICATION

In this simulation, a calculator was implemented. The variables for the calculator were defined and the Fortran statements were entered.

The calculator block was used to determine the product composition in the decomposition reactor. Table 2.7 shows the definition of the import variables using Streams created in the Calculator.

Table 2.7: Definition of the import variables for the Calculator block

Variable Name	Type	Stream	Substream	Component	Attribute	Elements
WATER	Compattr-Var	Feed	NC	BIOMASS	PROXANAL	1
ULT	Compattr-Vec	Feed	NC	BIOMASS	ULTANAL	-

The definition of the export variables using the Blocks category is listed in Table 2.8.

Table 2.8: Definition of the export variables for the Calculator 1

Variable Name	Type	Block	Variable	ID1	ID2
H_2O	Block-Var	DECOM	MASS-YIELD	H_2O	MIXED
ASH	Block-Var	DECOM	MASS-YIELD	ASH	NC
C	Block-Var	DECOM	MASS-YIELD	C	CISOLID

H_2	Block-Var	DECOM	MASS-YIELD	H_2	MIXED
N_2	Block-Var	DECOM	MASS-YIELD	N_2	MIXED
CL_2	Block-Var	DECOM	MASS-YIELD	CL_2	MIXED
S	Block-Var	DECOM	MASS-YIELD	S	MIXED
O_2	Block-Var	DECOM	MASS-YIELD	O_2	MIXED

Here ID1 stands for the corresponding components. ID2 stands for the classification of the component.

The Fortran statements from (Sun, 2014):

```
H20 = WATER/100
ASH = ((1 - WATER / 100)) * ULT (1) / 100
C = ((1 - WATER / 100)) * ULT (2) / 100
H2= ((1 - WATER / 100)) * ULT (3) / 100
N2 = ((1 - WATER / 100)) * ULT (4) / 100
CL2 = ((1 - WATER / 100)) * ULT (5) / 100
S = ((1 - WATER / 100)) * ULT (6) / 100
O2 = ((1 - WATER / 100)) * ULT (7) / 100
```

2.9 PROCESS DESCRIPTION

Since Aspen Plus does not have a specific gasifier model available for use, this research work models a dual fluidized-bed gasifier which breaks the entire process down into discrete blocks that can be replicated using Aspen Plus current models. The simulation process's flowsheet is displayed in Figure 2.1.

In this simulation, coconut shell biomass is introduced into the process as a non-conventional component via the feed block. The feed then enters the DECOMP reactor, which decomposes the biomass into conventional components based on its ultimate and proximate analysis. A calculator block is used to determine the yield of the components and is employed to control the decomposition yield. The decomposed stream flows into a PYRO reactor representing the pyrolysis process, where further break down into light gases (CO, CO_2, H_2, CH_4) and solid char (carbon). The stream passes into a splitter (SPLITTER), where it is separated into a gas stream (GAS) and a solid stream (SOLID). The solid stream contains an unreacted char, which is sent to

SEP1 (SEPERATOR) for further separation of ASH and CARBON (char for gasification). Steam is introduced via the STEAM stream which is used as the gasifying agent for this research and a calculator block was also introduced to calculate the steam to be input in the mixer. In the MIXER, the separate gas stream from GAS, char from CARBON, and STEAM are mixed to form a product gas (GAS-OUT), which becomes the feed to the oxidation zone (OXI). The OXI reactor simulates partial oxidation or combustion of part of the char and volatiles to generate the required heat for the downstream reduction zone (RED). The output from OXI (OXI-OUT) enters the RED reactor, which represents the reduction (gasification) step. In this zone, endothermic gasification reactions occur, generating syngas rich in H_2, CO, CO_2, and CH_4. The output gas stream RED-OUT is then cooled in the COOLER to a suitable temperature before separation. It is then fed to a separator (SEP2) where hydrogen (H_2) is separated as a product stream (H_2), while other gases exit via OG stream.

In this simulation of the gasification process of coconut shells, the following assumptions were made based on the characteristics of Aspen Plus and the kinetic model that was used:

- Process operates in a steady state.
- Operation takes place under atmospheric pressure, and all pressure losses are neglected.
- Char is 100% carbon.
- Steam is used as the gasifying agent
- Peng-Robinson equation of state was selected as the kinetic package for all processes.
- Tar formation is significantly reduced in the process, so it is neglected during the simulation.
- Ash comes from the biomass is considered as inert; it does not react with other components.
- All elements that compose the biomass yield into Char, H_2, O_2, N_2 , Cl_2, S.

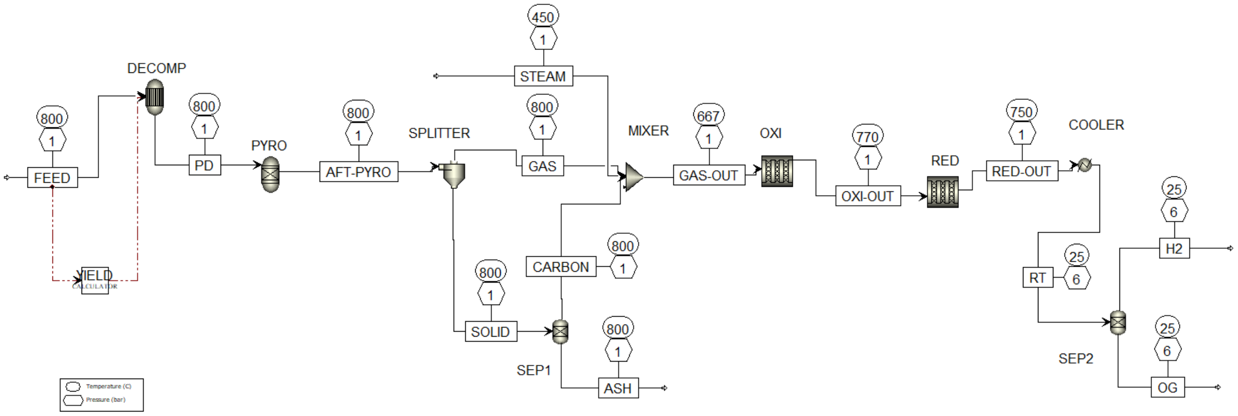


Figure 2.1: The flowsheet of coconut shell simulation

2.10 SENSITIVITY ANALYSIS

Sensitivity analysis is a technique for determining the way in which changes input variables determine the output process of the model. This is the property of Aspen Plus with the choice of design specifications (Singh et al., 2022). Sensitivity analysis was conducted to analyze the impact of the most important operating parameters on the gasification process performance with a focus on the composition of the reduction block product. The operating parameters applied were operating pressure, temperature, and steam flow rate. Each variable was systematically varied within a defined range while keeping syngas (H_2,CO, CO_2 and CH_4) composition constant, to know its influence on syngas yield and composition. This approach enabled the identification of optimal process conditions and provided insights into the relative impact of each parameter on system performance.

2.11 ECONOMIC ANALYSIS

The economic analysis was carried out within Aspen Process Economic Analyzer (APEA) by systematically configuring the economic interface to reflect realistic cost conditions. The procedure began by selecting the “Economics” tab from the toolbar, which provides access to the costing environment. The “Stream Price” option was then used to assign specific cost values to each material in the input and output streams, based on data from the literature. Next, the “Process Utilities” section was configured to define the utility scenarios relevant to the gasification process, followed by specifying the currency and costing details under the “Cost Options” menu. Finally, the “Auto-Evaluate” feature was enabled, allowing the software to automatically perform a comprehensive techno-economic evaluation of the process.

The economic analysis plays a pivotal role in the development and commercialization of the coconut shell gasification process. This analytical approach is used for identifying key economic drivers and gaining insights into factors influencing commercial success. The economic analysis for coconut shell gasification process was performed using Aspen Process Economic Analyzer (APEA), inputting cost data for various process streams to evaluate the system financial feasibility. Stream prices were assigned to key material flows, including biomass feed (coconut shell), steam (steam) as the feed streams for the stream price and hydrogen (H_2), other gases (OG), and ash as the product streams for the steam price based on their prices sourced from relevant literatures. The pricing basis was defined per unit mass ($/kg) and entered directly into the software economics interface to ensure accuracy in the simulation of cost-related outputs.

The feedstock cost for coconut shell was set at \$0.15/kg (Zhao et al., 2018), while the utility steam used for gasification was priced at \$0.04617/kg (Salimi et al., 2023). The product hydrogen stream was valued at \$5/kg (Majewski et al., 2023), reflecting market rates for high-purity H_2, and other gases (OG) was priced at \$0.131892/kg which included gases such as CO, CO_2, CH_4, H_2O, S, C, and N_2 (Morgenthaler et al., 2020, Kildahl et al., 2020, Khosravi et al., 2023, Vásquez-Lavín et al., 2020, Medhat et al., 2024). Ash, treated as a by-product or disposal stream, was assigned a cost of \$0.077/kg (Hope et al., 2017).These cost inputs were used to simulate the full economic profile of the process, resulting in key financial indicators such as Capital Cost, Annual Operating and Raw Material Costs, Product Sales, Utility Cost, Equipment Cost, Payback Period, and Rate of

Return. The simulation allowed for a comprehensive evaluation of the techno-economic viability of coconut shell gasification under the defined operating conditions and market assumptions.

Chapter 3

RESULTS AND DISCUSSION

3.1 CHARACTERIZATION OF SOLID COCONUT SHELL WASTE

The characterization was carrier out by doing ultimate, proximate and sulfur analysis of the coconut shell sample.

- **Ultimate analysis**

Table 3.1: Experimental data of coconut Shell for proximate analysis

Ultimate Analysis	Results (%wt)	Methods
Moisture content	0.94	TGA701 Thermogravimetric Analyzer
Ash	1.20	DIN EN ISO 21656 (2021-06) Verfahren A
Volatile matter	97.43	TGA701 Thermogravimetric Analyzer
Fixed carbon	0.43	TGA701 Thermogravimetric Analyzer

- **Proximate analysis**

Table 3.2: Experimental data of coconut Shell for ultimate analysis

Ultimate Analysis	Results (%wt)	Methods
Ash	1.2	DIN EN ISO 21656 (2021-06) Verfahren A
Carbon	49.4	DIN EN ISO 21663 (2021-03)
Hydrogen	5.78	DIN EN ISO 21663 (2021-03
Nitrogen	0.160	DIN EN ISO 21663 (2021-03)
Chlorine	0.04	Calculation
Sulfur	0.02	DIN EN 15408 (2011-05)
Oxygen	43.4	DIN 51733 (2016-04)

- **Sulfur analysis**

Table 3.2: Experimental data of coconut shell for sulfur analysis

Sulfur analysis (dry basis)	Biomass	Ash
Pyritic	0	0
Sulfate	0	0
Organic	0.02	0

3.2 BIO-HYDROGEN SIMULATION RESULTS IN MOLE FRACTION FOR MY MODEL COMPARED TO PINEWOOD

The result of my model was compared with an experimental result from Yu et al., 2019. As shown in Table 3.3.

Table 3.3: Result of my model compared with an article Yu et al., 2019.

Gas	My Model	Experimental Model	Absolute Difference
H_2	0.304765	0.274	0.030765
CO	0.264351	0.252	0.012351
CO_2	0.0177414	0.020	0.0022586
CH_4	0.00643964	0.090	0.08356036

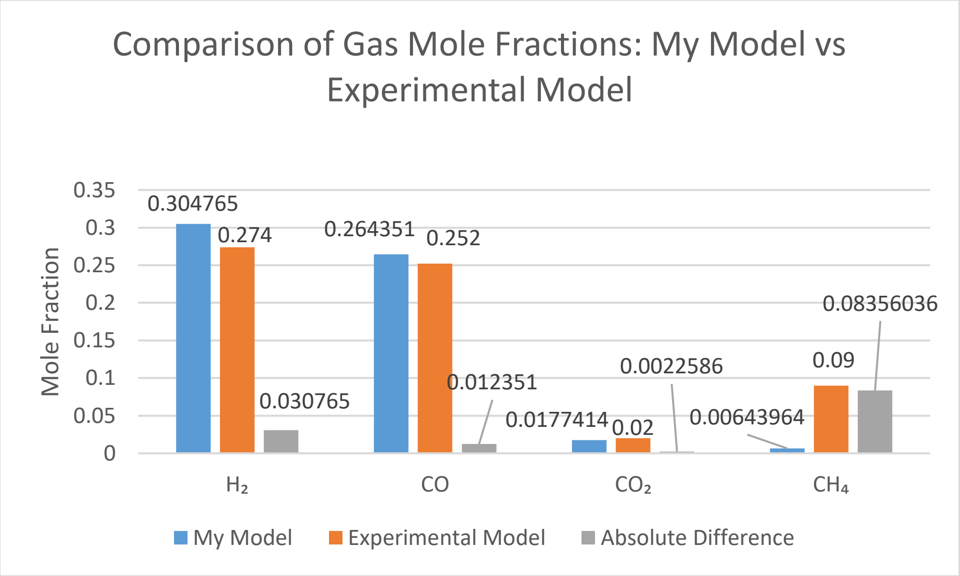


Figure 3.1 The comparison of gas mole fraction for my model compared to pinewood

- **The Root Mean Square Error (RMSE)**

The accuracy of the model is checked by comparing predicted gas composition from the proposed model with experimental results. The error in prediction is estimated with statistical parameter of root mean square error (RMSE) value.

RMSE = $\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y_i})^2}$ from (Rosyadi et al., 2024).

RMSE = $\sqrt{\frac{(0.304765-0.274)^2+(0.264351-0.252)^2+(0.0177414-0.020)^2+(0.00643964-0.090)^2}{4}}$

RMSE = $\sqrt{0.00202162}$

RMSE = 0.0449

- **BIO-HYDROGEN SIMULATION RESULTS IN MOLE FRACTION FOR MY MODEL COMPARED TO WOOD CHIPS**

The result of my model was compared with an Experimental results from Agu et al., 2019. As shown in Table 3.4.

Table 3. 4: Result of my model compared with an article Agu et al., 2019.

Gas	My Model	Experimental Model	Absolute Difference
H_2	0.304765	0.35	0.045235
CO	0.264351	0.22	0.044351
CO_2	0.0177414	0.13	0.1122586
CH_4	0.00643964	0.03	0.02356036

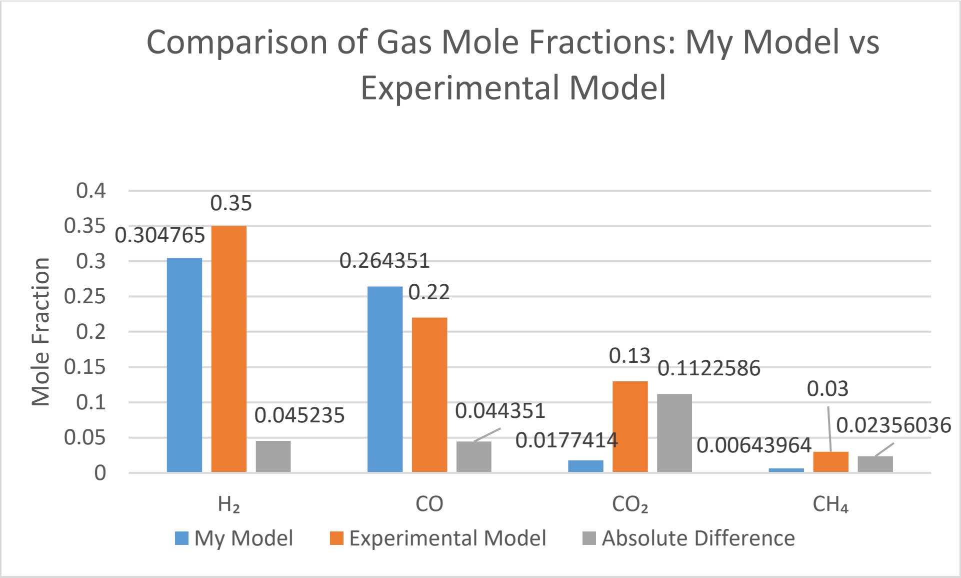


Figure 3.2: The comparison of gas mole fraction for my model compared to wood chips

- **The Root Mean Square Error (RMSE)**

The accuracy of the model is checked by comparing predicted gas composition from the proposed model with experimental results. The error in prediction is estimated with statistical parameter of root mean square error (RMSE) value.

RMSE = $\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \widehat{y_i})^2}$ from Rosyadi et al., 2024.

$$\text{RMSE} = \sqrt{\frac{(0.304765-0.35)^2+(0.264351-0.22)^2+(0.0177414-0.13)^2+(0.00643964-0.03)^2}{4}}$$

$$\text{RMSE} = \sqrt{0.004292575}$$

RMSE = 0.0655

3.3 SENSITIVITY ANALYSIS

Sensitivity analysis for coconut shell biomass gasification was carried out to study the effect of coconut shell flow rate, steam flow rate and the effect of temperature on the yield of products component compositions. The results obtained from the sensitivity analysis are presented in figures below.

- **EFFECT OF PRESSURE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)**

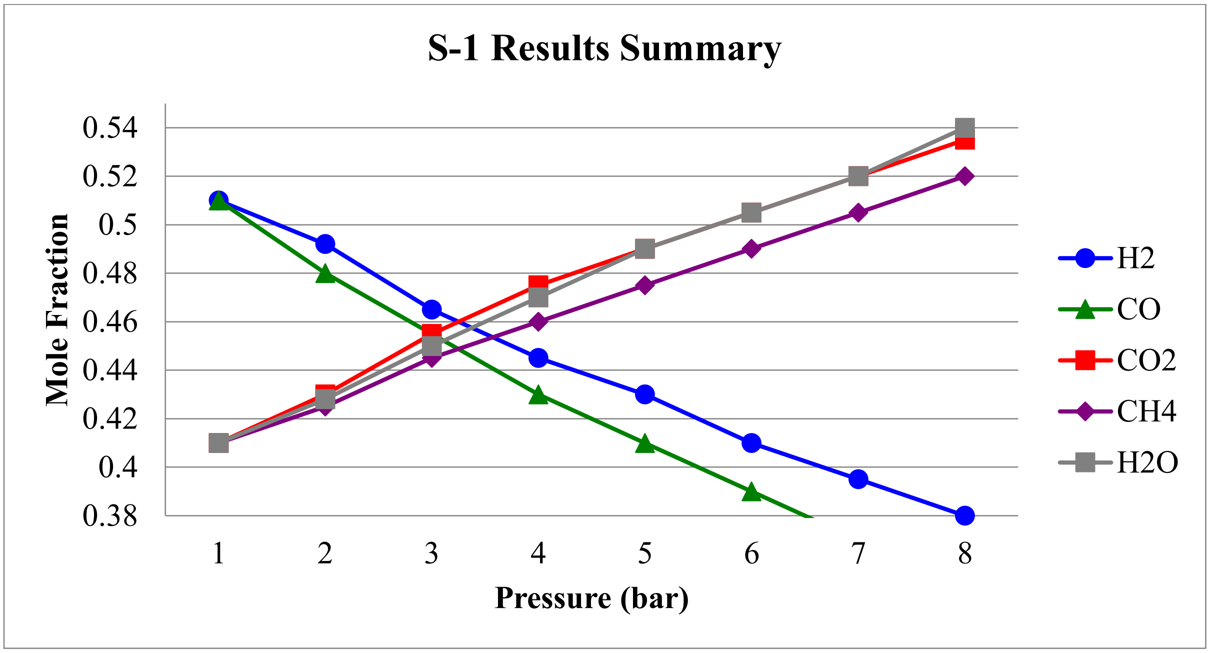


Figure 3.3: Effect of pressure on yield of product composition in reduction reactor (RED-OUT)

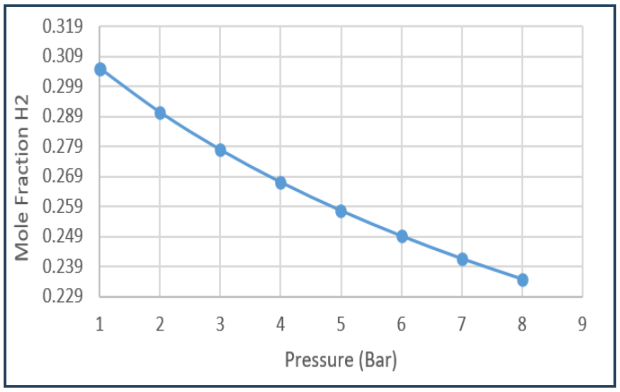


Figure 3.4: Effect of pressure on H_2

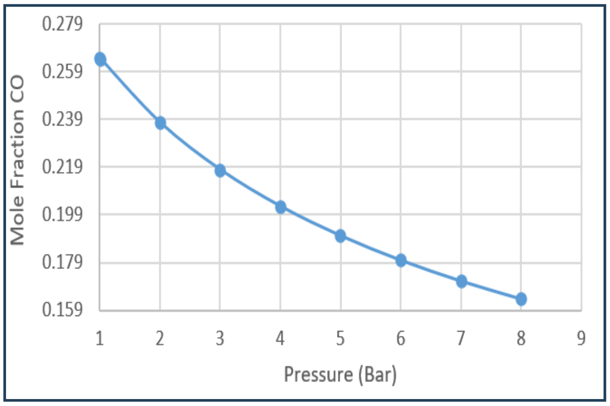


Figure 3.5: Effect of pressure on CO

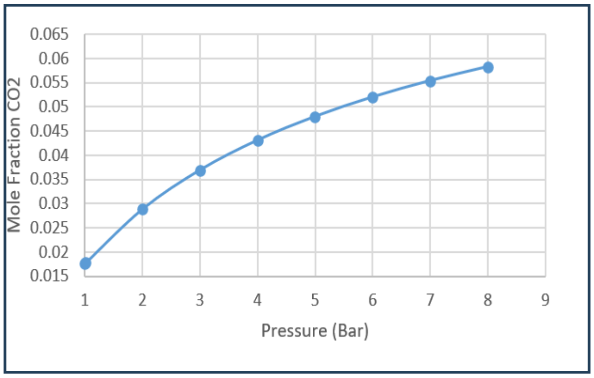


Figure 3.6: Effect of pressure on CO_2

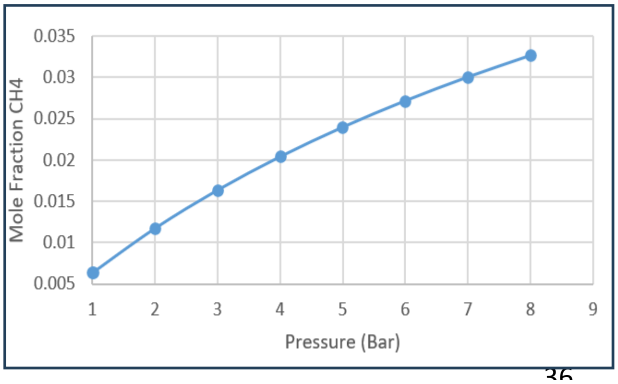


Figure 3.7: Effect on pressure on CH_4

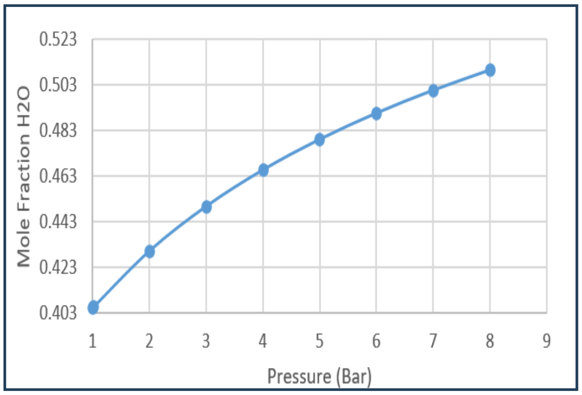


Figure 3.8 Effect of pressure on H_2O

- **EFFECT OF STEAM FLOW RATE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)**

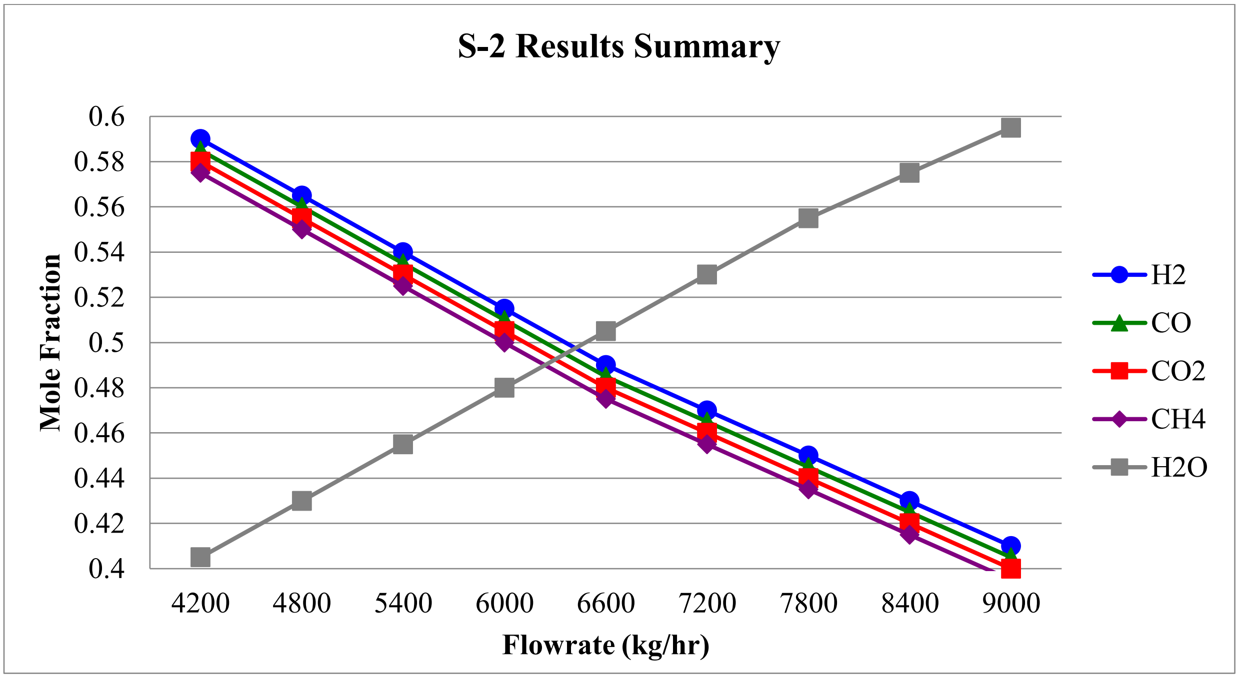


Figure 3.9: Effect of steam flow rate on yield of product composition in reduction reactor (RED-OUT)

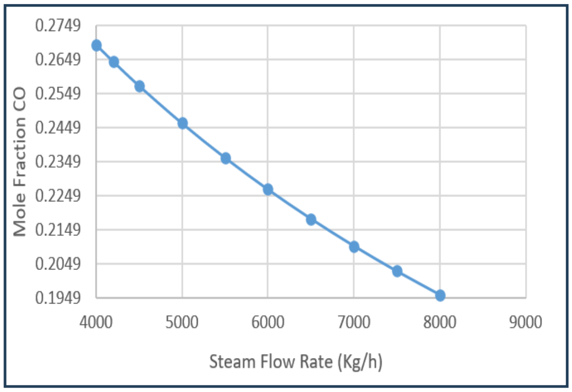


Figure 3.10: Effect of steam flow rate on CO

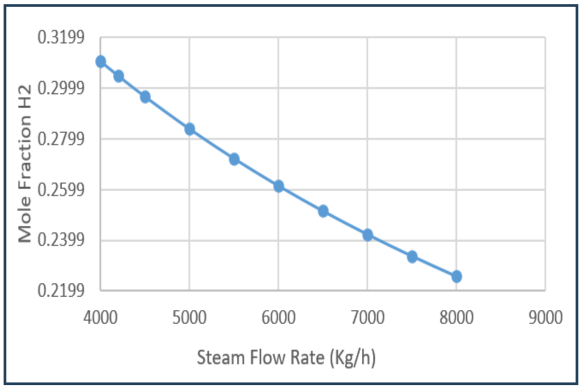


Figure 3.11: Effect of steam flow rate on H_2

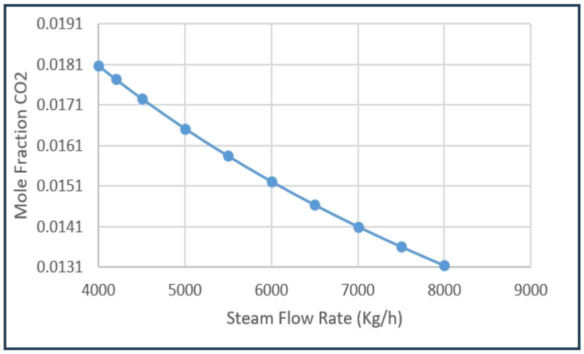


Figure 3.13: Effect of steam flow rate on CO_2

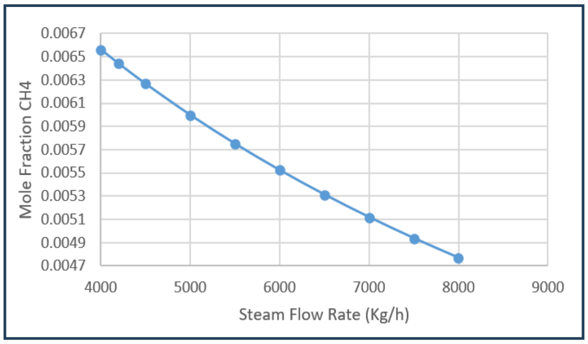


Figure 3.12: Effect of steam flow rate on CH_4

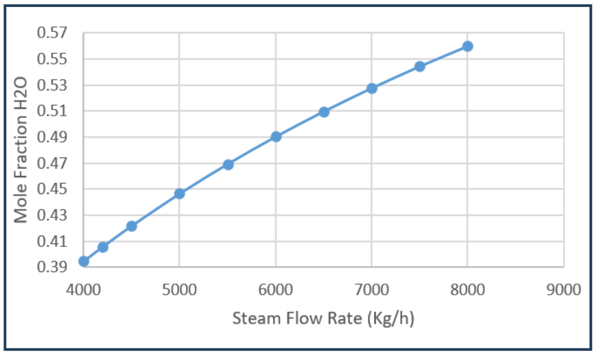


Figure 3.14: Effect of steam flow rate on H_2O

- **EFFECT OF TEMPERATURE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)**

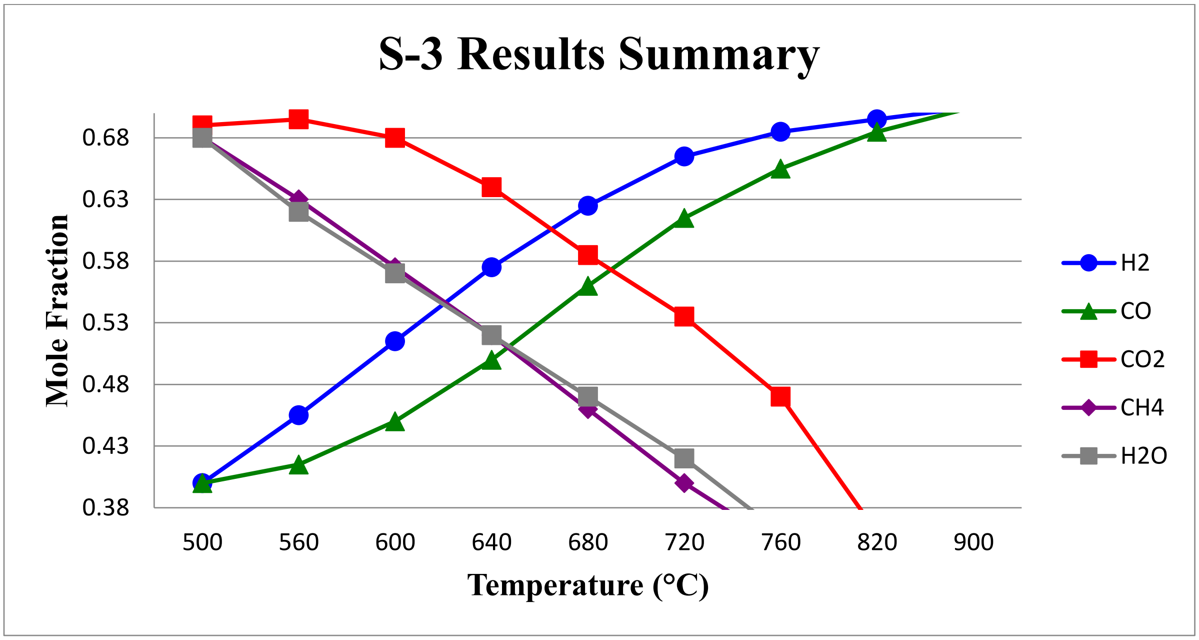


Figure 3.15: Effect of temperature on yield of Product composition in reduction reactor (RED-OUT)

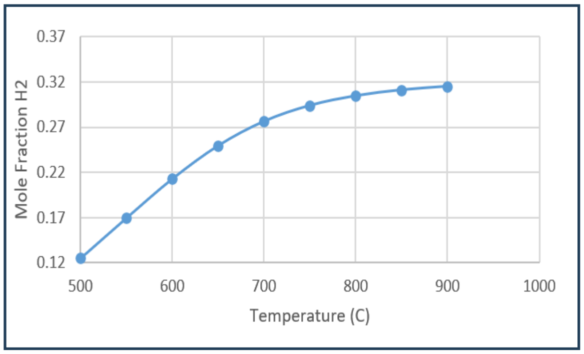


Figure 3.16: Effect of temperature on H_2

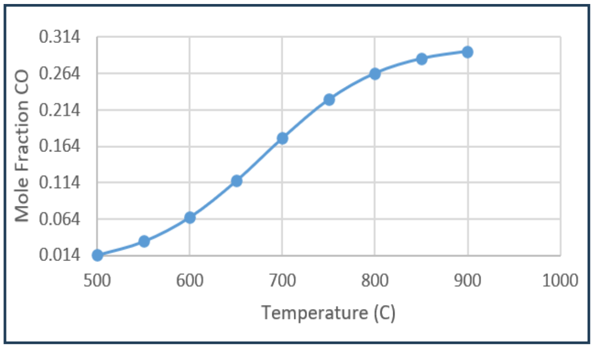


Figure 3.17: Effect of temperature on CO

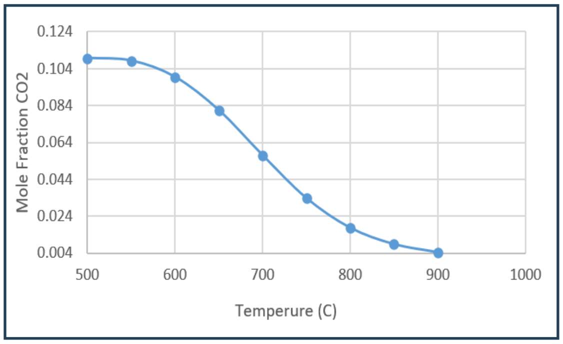


Figure 3.18: Effect of temperature on CO_2

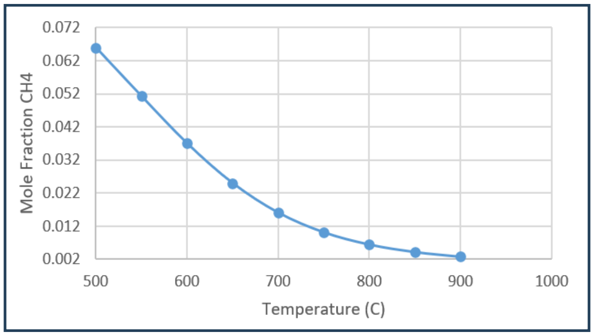


Figure 3.19: Effect of temperature on CH_4

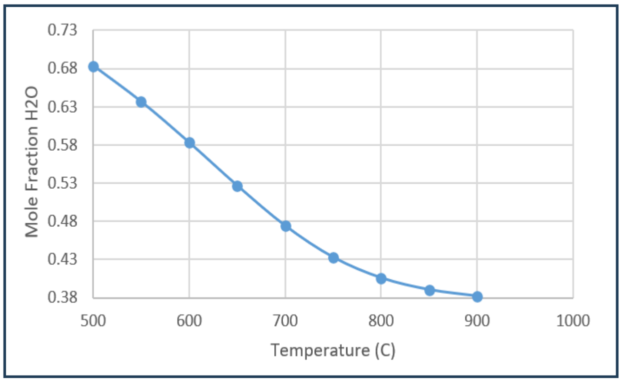


Figure 3.20: Effect of temperature on H_2O

3.4 ECONOMIC ANALYSIS

Table 3.3 below shows the economic analysis done by Aspen Plus using the Aspen Process Economic Analyzer (APEA).

Table 3.1: Economic analysis of coconut shell gasification from Aspen Process Economic Analyzer (APEA)

Metric	My Aspen Result
Capital Cost	USD 5.84 million
Operating Cost/year	USD 12.92 million
Raw Material Cost/year	USD 10.90 million
Product Sales/year	USD 28.53 million
Payback Period	7.04 years
Rate of Return	20%
Utility Cost/year	USD 199,017
Equipment Cost	USD 353,600

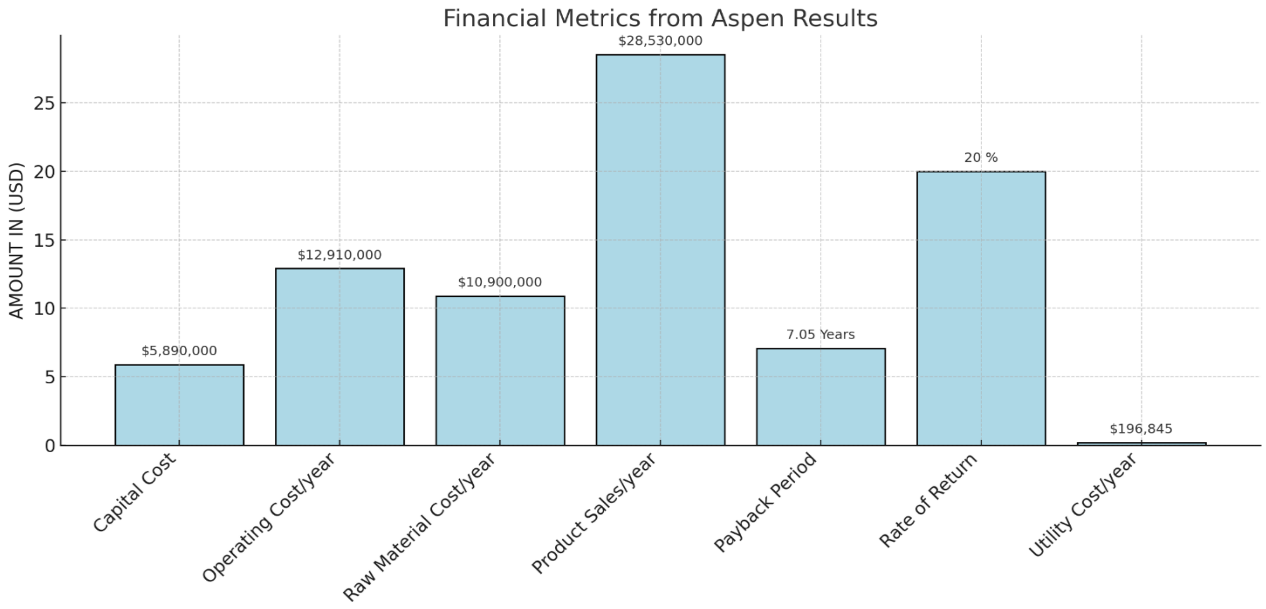


Figure 3.21: Economic analysis of coconut shell gasification from Aspen Process Economic Analyzer (APEA).

3.5 DISCUSSION

3.5.1 BIO-HYDROGEN SIMULATION RESULTS IN MOLE FRACTION FOR MY MODEL COMPARED TO PINEWOOD

In this study, the developed kinetic model was validated against experimental data in mole fraction reported by Yu et al. (2019) in table 3.3. The study is on gasification of pinewood in a downdraft gasifier using a detailed kinetic approach. The purpose of this comparison was to assess the predictive capability of the model, particularly in estimating syngas composition under similar process conditions. The model closely matched their reported syngas values for major gases. For hydrogen (H_2) and carbon monoxide (CO), the predicted mole fractions were 0.3048 and 0.2644, compared to experimental values of 0.274 and 0.252 respectively, producing a minor absolute difference of 0.0308 H_2 and 0.0124 CO. The predicted value for Carbon dioxide (CO_2) is 0.0177 compared to the experimental result of 0.020 with an absolute difference of 0.0023. However, methane (CH_4) was significantly underpredicted at 0.0064, compared to the experimental value of 0.090 with an absolute difference of 0.0836. This underestimation is consistent with previous findings that methane is particularly sensitive to assumptions in tar formation, cracking, and reaction temperature in kinetic modeling frameworks (Yu et al., 2019).

To quantify the overall model accuracy, the Root Mean Square Error (RMSE) was calculated using the expression proposed by Rosyadi et al. (2024), yielding an RMSE of 0.0449. This low RMSE indicates strong predictive performance, when benchmarked against (Yu et al., 2019).

3.5.2 BIO-HYDROGEN SIMULATION RESULTS IN MOLE FRACTION FOR MY MODEL COMPARED TO WOOD CHIPS

In this study, the developed kinetic model was further validated against experimental mole fraction data reported by Agu et al. (2019) in table 3.4, who investigated the steam gasification of wood chips in a bubbling fluidized bed reactor using a detailed one-dimensional model. The aim of this comparison was to examine the syngas composition under different feedstock and operational conditions.

The predicted mole fractions for hydrogen (H_2) and carbon monoxide (CO) were 0.3048 and 0.2644, respectively, compared to experimental values of 0.35 for H_2 and 0.22 for CO. The resulting absolute differences of 0.0452 and 0.0444 indicate that the model approximates the behavior of key gas composition, even with differences in feedstock and reactor type. The level of agreement for H_2 and CO suggests that the model kinetic parameters are generally robust for major syngas constituents. The model underpredict carbon dioxide (CO_2) with a mole fraction of 0.0177, whereas the experimental value reported by Agu et al. (2019) was significantly higher at 0.13, giving an absolute deviation of 0.1123. This variation is due to the specific characteristics of the feedstock used wood chips which have different reactivity and ash content compared to coconut shell. Other factors that can influence this change are the steam to biomass ratio and temperature distribution within the reactors which can lead to the underprediction of the value of carbon dioxide (CO_2)). In the case of methane (CH_4)), the model predicts a value of 0.0064, compared to the experimental value of 0.03, giving a deviation of 0.0236. This underestimation is not surprising, as CH_4 formation is strongly influenced by tar cracking reactions and thermal conditions factors that are not fully captured in simplified kinetic models like the one used in this study. Similar challenges have also been reported by Agu et al. (2019), where accurately predicting methane remained a limitation.

To evaluate the overall accuracy of the model, the Root Mean Square Error (RMSE) was calculated based on the method described by Rosyadi et al. (2024). The RMSE is 0.0655 across the four gas compositions. Although this value is slightly higher than what was obtained in the previous comparison with Yu et al. (2019), it still falls within a reasonable range for gasification modeling, especially considering the differences in reactor configuration and feedstock properties. This indicates that the model remains useful for practical applications, but improvements are still needed to better represent certain reactions and gas composition under fluidized bed conditions.

3.5.3 EFFECT OF PRESSURE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)

This study shows in figure 3.3, the influence of pressure variation 1–8 bar on the mole fraction of syngas components H_2, CO, CO_2, CH_4, and H_2O in the reduction block of the coconut shell gasification model using steam as the gasifying agent. As shown in figure 3.3, increasing pressure leads to a noticeable decline in the mole fractions of hydrogen (H_2) and carbon monoxide (CO), while the concentrations of carbon dioxide (CO_2), methane (CH_4), and moisture (H_2O) progressively increase.

At 1 bar, H_2 and CO mole fractions are approximately 0.305 and 0.265 respectively, as pressure increases to 8 bar, these values fall to about 0.230 and 0.160. This inverse relationship aligns with Le Chatelier's principle, where increased pressure shifts the equilibrium toward reactions with fewer gas-phase moles, thus favoring the formation of CH_4 and CO_2 over H_2 and CO. In contrast, CH_4 and CO_2 increase from 0.005 and 0.170 to 0.035 and 0.240 respectively, indicating that methanation ($C + 2H_2 \rightarrow CH_4$) and the water–gas shift reaction ($CO + H_2O \rightarrow CO_2 + H_2$) are favored under elevated pressure.

These trends are consistent with the findings of Zhang et al. (2023), who conducted a pressure sensitivity study on cow dung biomass gasification. Their model showed that increasing pressure from 1 atm to 9 atm led to a decline in H_2 from 55.8% to 47.2% and CO from 28.8% to 24.1%, while CO_2 and CH_4 increased significantly CO_2 from 15.2% to 21.0%, CH_4 from 0.003% to 7.79%. Their interpretation attributes the increase in CH_4 to enhanced methanation and the decrease in H_2 to backward shifts in the water–gas reaction ($C + H_2O \rightarrow CO + H_2$) under pressure.

3.5.4 EFFECT OF STEAM FLOW RATE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)

This study assessed the sensitivity of product gas composition to varying steam flow rates from 4200–9000 kg/h in the reduction section of a coconut shell gasification model. The results in figure 3.4, demonstrate a clear inverse relationship between steam flow rate and the mole fractions of H_2, CO, CO_2, and CH_4, while the mole fraction of unconverted H_2O increases proportionally with steam input.

At lower steam flow rates 4200 kg/h, hydrogen (H_2) exhibits a mole fraction of approximately 0.305, carbon monoxide (CO) peaks at 0.265, and carbon dioxide (CO_2) is around 0.210. However, as steam flow increases to 9000 kg/h, the mole fractions of these gases decline sharply, reaching approximately 0.230 for H_2, 0.180 for CO, and 0.185 for CO_2. A similar trend is observed for methane (CH_4), which also decreases due to enhanced steam reforming reactions consuming CH_4. In contrast, H_2O increases from 0.41 to nearly 0.60, indicating increased dilution and incomplete conversion of the injected steam.

These findings align with the experimental results reported by Ponzio et al. (2006), who examined steam-rich gasification in a high-temperature updraft fixed-bed reactor. Their study showed that increasing steam content initially promotes H_2 formation via steam reforming and the water–gas shift reaction. However, beyond a certain threshold, excessive steam leads to gas dilution, a drop in reaction temperature, and a reduction in the concentration of key syngas components (H_2, CO, CH_4). Specifically, they observed a decline in CO and CH_4 with increasing steam input and a slight decrease in H_2 beyond optimal steam conditions.

The results from both the model and the experimental data support the understanding that there exists an optimal steam flow rate, above which the benefits of steam-enhanced reactions are offset by thermal and dilution effects. Excess steam reduces residence time and lowers the partial pressure of reactive species, suppressing endothermic reactions such as Boudouard ($C + CO_2 \rightarrow 2CO$) and steam reforming ($CH_4 + H_2O \rightarrow CO + 3H_2$).

3.5.5 EFFECT OF TEMPERATURE ON YIELD OF PRODUCT COMPOSITION IN REDUCTION REACTOR (RED-OUT)

The sensitivity analysis of temperature on syngas composition in the reduction reactor (RED-OUT) was analyzed and shows clear trend that aligns with Zhang et al. (2023) in figure 3.5.

This study shows that the yield of hydrogen (H_2) and carbon monoxide (CO) increases with temperature, while carbon dioxide (CO_2), methane (CH_4), and steam (H_2O) decreases. At 500 °C, H_2 and CO mole fractions begin relatively low but progressively increase to reach their peak at around 900 °C, reaching values near 0.07 and 0.065 respectively. Conversely, CO_2 decreases from 0.07 at lower temperatures to below 0.01 at 900 °C. This behavior corresponds with the endothermic nature of the Boudouard reaction ($C + CO_2 \rightarrow 2CO$) and steam-reforming reactions ($C + H_2O \rightarrow CO + H_2$), which are promoted by higher temperatures.

The experimental work from (Zhang et al., 2023) reported similar behavior in their cow dung gasification model, where increasing the gasification temperature from 700 °C to 1100 °C led to a rise in H_2 (from 44.9% to 54.4%) and CO (from 9.7% to 34.1%) content, and a reduction in CO_2 (from 32.5% to 11.6%) and CH_4 (from 12.9% to near-zero). These changes are attributed to shifts in favor of endothermic reactions at high temperatures, especially the Boudouard and water–gas reactions (R3, R4, R5). In both models, methanation and water-gas shift reactions, which are exothermic, are suppressed with increasing temperature, explaining the decrease in CH_4 and CO_2.

The work from (Zhang et al., 2023) observed a maximum H_2 concentration around 900 °C before a slight decline, likely due to enhanced water–gas shift reaction consumption of H_2 and reverse methanation at higher temperatures. This aligns with the H_2 seen in my results beyond 850 °C.

3.5.6 ECONOMIC ANALYSIS

The economic analysis of the coconut shell gasification process, as simulated in Aspen Plus and evaluated using Aspen Process Economic Analyzer (APEA), demonstrates promising financial viability for commercial-scale deployment as shown in table 3.3. The total capital cost of the plant was estimated at USD 5.89 million, with annual operating and raw material costs of USD 12.91 million and USD 10.9 million, respectively. Despite these substantial expenditures, the system yielded an impressive annual product revenue of USD 28.53 million, resulting in a payback period of 7.05 years and a rate of return of 20%, which falls within acceptable industry standards for renewable energy investments. These findings are consistent with those reported by Kottakalathil et al. (2025), who performed a techno-economic assessment of coconut shell bioenergy production using Aspen Plus and APEA. Their model, although based on a smaller-scale configuration, showed similar financial performance, reporting an internal rate of return of 24.1% and a payback period of 4.5 years, which they attributed to reduced capital input. The consistency in profitability indicators between the two studies underscores the scalability of coconut shell gasification as a viable bioenergy solution. Moreover, the relatively low utility cost in this study USD 196,845/year further enhances its attractiveness by reflecting operational energy efficiency. The economic metrics validate the commercial potential of the simulated process and align with previous experimental findings that demonstrate favorable outcomes under optimized thermochemical and financial parameters, thereby reinforcing the robustness and applicability of the Aspen-based economic modeling approach from (Kottakalathil et al., 2025).

Chapter 4

CONCLUSION AND PERSPECTIVES

4.1 Conclusions

This study established that coconut shell waste in Sierra Leone holds significant potential as a feedstock for sustainable bio-hydrogen production through thermochemical gasification. The Aspen Plus kinetic model produced syngas compositions that closely aligned with experimental results, especially for hydrogen and carbon monoxide, while maintaining acceptable error margins for other gases. The sensitivity analysis revealed that temperature, pressure, and steam flow rate substantially influence hydrogen yield and overall syngas quality, with higher temperatures favoring hydrogen and carbon monoxide formation. The economic evaluation confirmed the feasibility of the process, indicating an attractive payback period and rate of return. These findings validate the initial hypotheses that gasification of coconut shells can contribute meaningfully to renewable energy generation, reduce greenhouse gas emissions, and provide a sustainable solution to waste management challenges in Sierra Leone.

4.2 Perspectives

Future research should aim to broaden the scope of this work through experimental validation at pilot or industrial scales, which would strengthen the reliability of the model predictions. Further improvements could include:

- Incorporating advanced kinetic mechanisms to better account for methane formation and tar cracking.
- Explore alternative gasifying agents such as oxygen or air for enhanced hydrogen yields. Integrating carbon capture and storage technologies into the process design could amplify the environmental benefits by reducing residual Carbon dioxide emissions.
- Conducting comprehensive life-cycle assessments and techno-policy analyses would provide greater insight into the long-term sustainability and socio-economic impacts of large-scale adoption.

By deepening these aspects, this research can serve as a foundation for practical renewable energy strategies that transform agricultural waste into valuable energy resources, ultimately supporting Sierra Leone’s transition toward a low-carbon future.

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