



Process Simulation of Steam Reforming of Different Feedstocks

by

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Preface

The research contained in this thesis was completed by the candidate while based in the Discipline of Engineering, School of Chemical Engineering of the College of Agriculture, Engineering and Science, University of KwaZulu-Natal, Howard College, Durban, South Africa. The research was financially supported by the University of Kwa-Zulu Natal: Strategic Funds and Fee Remission as well as supervisor's cost centre.

The contents of this work have not been submitted in any form to another university and, except where the work of others is acknowledged in the text, the results reported are due to investigations by the candidate.

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Abstract

In response to environmental challenges such as waste disposal, natural resource depletion and climate change there has been an increasing focus on extracting value from different waste streams and on alternative feedstocks for chemical and energy industry. Steam reforming has the potential to convert different waste streams such as biomass waste, waste plastics and waste tyres to synthesis gas (syngas). Syngas can be used for production of liquid fuels via the Fischer-Tropsch process, Combined Heat and Power (CHP) generation as well as production of important industrial chemicals such as Hydrogen, Ammonia and Methanol.

The objective of this work was to model and simulate the steam reforming process for different feedstocks such as biomass waste, waste plastics and waste tyres using ASPEN Plus. To do so, a non-stoichiometric restricted equilibrium-based model was developed using the minimisation of Gibbs free energy method. The model results were compared with experimental data from the literature for steam reforming of wood chips and the model result agreed with experimental data thus validating the model.

The key operating parameters such as steam temperature, steam to feed ratio, gasifier temperature, combustion air temperature and combustion air to feed ratio were varied using the sensitivity analysis tool on ASPEN Plus. The effect of changing the mentioned variables on syngas composition, syngas Lower Heating Value (LHV) and Cold Gasification Efficiency (CGE) was studied and analysed. The sensitivity analysis results were discussed for only 3 out of 15 feedstock considered which are Wood Chips, Sugarcane Bagasse and Rice Husk.

The results from the model indicated that syngas produced from steam reforming of Wood Chips, Sugarcane Bagasse, Black Liquor and Pig Manure has a H_2/CO ratio of 1,81 – 2,20 which is suitable for production of liquid fuels via the Fischer-Tropsch process without adjustment. Furthermore, the model results indicated that Food Waste, Municipal Solid Waste, Waste Plastics (PP), Waste Plastics (PE), Waste Tyres and Coal produced syngas with the poorest quality as indicated by low H_2 and CO content, respectively. The reason for poor syngas quality is high moisture content, high ash content and low fixed carbon as indicated by the proximate analysis of the respective feedstock. Moreover, the feedstocks that produced the poorest syngas quality has high LHV due to the presence of CH_4 in significant quantity. High LHV makes them suitable for use in energy applications such as Combined Heat and Power (CHP) and Integrated Gasification Combined Cycle (IGCC) as opposed to chemical production.

The results from the sensitivity analysis indicated that for the case of Wood Chips and Rice Husk steam reforming, increasing steam temperature leads to an increase in the concentration of H₂ and CO but a decrease in CO₂ and CH₄. Furthermore, an increase in steam temperature decreases the syngas LHV and increases the CGE for steam reforming of Wood Chips and Rice Husk, however, the syngas composition, syngas LHV and CGE remained almost unchanged with an increase in steam temperature for steam reforming of Sugarcane Bagasse. The optimal steam temperature for steam reforming of Wood Chips and Rice Husk was found to be 750 °C and 800 °C, respectively.

Furthermore, the results from the sensitivity analysis indicated that increasing steam to feed ratio increases H₂ and CO₂ but decreases CO and CH₄ concentration in syngas for steam reforming of Wood Chips, Sugarcane Bagasse and Rice Husk. In addition to this, it was noted that an increase in steam to feed ratio leads to a substantial decrease in syngas LHV and only a slight decrease in CGE for steam reforming of Wood Chips, Sugarcane Bagasse and Rice Husk. The optimal steam to feed ratio was found to be dependent on the desired syngas end use. If the desired syngas end use is industrial chemical production where H₂/CO ratio of ~ 2 is required, the optimal steam to feed ratio is 0,56, 0,72, and 0,43 for steam reforming of Wood Chips, Sugarcane Bagasse and Rice Husk, respectively. However, if the desired syngas end use is hydrogen production where a high H₂/CO ratio is required then the steam to feed ratio needs to be as high as possible

Moreover, sensitivity analysis results indicated that as the gasifier temperature is increased, both H₂ and CO increases while CO₂ and CH₄ decrease. Furthermore, LHV drops while CGE increase for steam reforming of all 3 feedstocks. The optimal gasifier temperature was found to be 867 °C, 923 °C, and 929 °C for steam reforming of Wood Chips, Sugarcane Bagasse and Rice Husk, respectively. The effect of combustion air temperature is the same as that of the gasifier temperature. The optimal combustion air temperature was found to be 641 °C, 641 °C, and 898 °C for Wood Chips, Sugarcane Bagasse and Rice Husk steam reforming, respectively. Lastly, the combustion air to feed ratio has a negative impact on syngas as indicated by a drop in both H₂ and CO as well as a drop in syngas LHV, hence it should be kept as low as possible.

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Several people/organisations deserve special acknowledgements for their direct/indirect contribution to making this work a success:

- My supervisor Prof Amir H. Mohammadi for providing me with an opportunity to conduct an interesting research project and arranging the project funding for me. Moreover, I am grateful for his professional opinions, instructive advice, and useful suggestions to my dissertation.
- Preyo Nayager of the University of Kwa-Zulu Natal (UKZN) for his assistance with the installation and periodic update of ASPEN Plus software on my PC.
- Fiverr & Facebook for providing a network to connect with ASPEN Plus users.
- Nkosikhona Myeza & Bonginkosi Ndwandwe for their assistance with transporting my laptop to the University for Updates on ASPEN Plus software.
- My son, Melokuhle for understanding my busy schedule while I was juggling with full time work, part time studies amidst single parenthood.
- Finally, God – The Almighty for providing me with strength, courage, bravery, and wisdom to undertake this project.

Dedication

This dissertation is dedicated to my late mom - Intomb'Ka Masineka (uMfanawendaba)

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Nomenclature

Abbreviations

CGE	Cold Gasification Efficiency
CHP	Combined Heat and Power
FC	Fixed Carbon
HV	Heating Value
ICGG	Integrated Gasification Combined Cycle
LHV	Lower Heating Value
PE	Polyethylene
PP	Polypropylene
Syngas	Synthesis Gas
VM	Volatile Matter

Subscripts

m	Stoichiometric coefficient
n	Stoichiometric coefficient
k	Stoichiometric coefficient

Units

kJ	Kilo Joule
C	Celsius
°	Degrees

kg	Kilogram
MJ	Mega Joule
Nm ³	Normal cubic meter

Letters and Expressions

%	Percentage
wt %	Weight Percentage
vol %	Volume Percentage

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Chapter 1 Introduction

1.1. Rationale and Justification

In response to environmental and sustainability challenges such as increasing climate change and depletion of fossil fuels, a quest for alternative feedstocks for chemical and energy production has been necessitated. Currently, solid waste is disposed of mainly by landfilling and incineration (Nahman, 2021). These waste disposal methods are unsustainable due to the harm that they cause to the environment (Sithole, 2017a). Environmental concerns associated with waste landfilling and incineration are space shortage, greenhouse gas emissions and leaching of toxic fluids to the surrounding ecosystem (Sithole, 2017b).

As a result of challenges posed by current waste disposals techniques such as incineration and landfill, there has been a need for a different, sustainable, environmentally friendly, and economically sound approach to waste handling such as conversion of different waste streams to energy and chemicals. Steam reforming is one technology that has the potential to produce energy and chemicals from different waste streams. As a result of this potential, steam reforming of different feedstocks has received increasing attention by researcher due to its technical and economic feasibility.

Steam reforming is a thermo-chemical process that converts carbonaceous feedstocks by reacting it with steam at high temperature to produce syngas (Kish, 2016). Syngas is comprised mainly of hydrogen and carbon monoxide, smaller amount of methane, carbon dioxide, nitrogen, and water (Kish, 2016). Usually, steam reforming is performed with fossil fuel feedstocks such as natural gas, crude oil, and coal. Steam reforming represents an alternative treatment of waste materials to produce syngas with higher energy and higher hydrogen content than syngas produced from gasification (Kish, 2016).

1.2. Aims

The main aims of this research were to:

- Develop an ASPEN Plus model for simulating the steam reforming process of different feedstocks using ASPEN Plus V11.
- And to verify the simulation results against experimental data from the literature.

1.3. Objectives

To achieve the above mentioned aims, the objectives of this research were to:

- Identify suitable feedstocks for use in the steam reforming process.
- Obtain proximate, ultimate and sulfanal analysis data for the selected feedstocks.
- Select a suitable physical property method for modelling of the steam reforming process using ASPEN Plus V11.
- Perform sensitivity analysis of different process variables which are: steam temperature, steam to feed ratio, gasifier temperature, combustion air temperature and combustion air to feed ratio on syngas compositions, syngas Lower Heating Values (LHV) and Cold Gas Efficiency (CGE).

1.4. Dissertation Outline/Structure

The body of this dissertation is divided into 6 separate chapters from the introductory chapter 1 to the last chapter where the dissertation is wrapped up on chapter 6. The description of the content of each chapter is outlined below:

Chapter 1: Introduces the topic of steam reforming of different feedstocks and covers the rationale, justification, research aims and objectives of the topic research topic.

Chapter 2: Delves into the literature review of steam reforming of different feedstocks. A detailed review is made on different reforming technologies, different feedstocks which are renewable and non-renewable for steam reforming process, feedstock analysis such as composition and thermodynamic

analysis, Heating Value (HV), Lower Heating Value (LHV) of syngas and Cold Gasification Efficiency (CGE). Moreover, a highlight of the most common uses of syngas such as production of ammonia, hydrogen and methanol, gas to liquid (GTL) as well as electricity generation is provided. The chapter concludes by providing an introductory overview on ASPEN Plus software, particularly relating to steam reforming process.

Chapter 3: Provides a detailed description of the methodology used to develop the ASPEN Plus simulation model which was used in this research. The chapter begins by providing a detailed process description of the flowsheet used on ASPEN Plus. After the detailed process description, a detailed explanation of the physical property methods selection, stream specification, block specification and calculator blocks used in the simulations is provided.

Chapter 4: Presents the results obtained from the study and compares them with experimental data from the literature to validate the developed model on ASPEN Plus. Moreover, the sensitivity of different process variables which are: steam temperature, steam to feed ratio, gasifier temperature, combustion air temperature and combustion air to feed ratio on syngas composition, syngas LHV and CGE is presented graphically.

Chapter 5: Discusses the meaning and implications of the results presented in the previous chapter. Furthermore, the reasoning behind the observations made in chapter 4 is provided as far as possible by making referring to chemical engineering fundamentals.

Chapter 6: Summarises major results and findings from the study carried out as part of the research that is presented in this dissertation. Following the conclusion of the research, a highlight on recommendations relating to the research topic were made. The recommendations part provides potential improvements on work that was conducted and suggestions regarding further studies that should be carried out to obtain more insight into the research topic.

Chapter 2 Literature Review

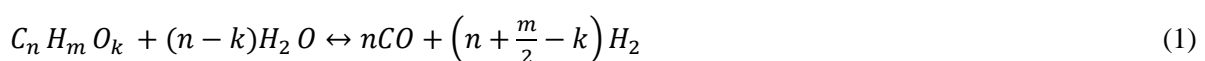
2.1 Reforming Technologies

Reforming is the widely used technology for converting carbonaceous feedstocks to synthesis gas commonly referred to as syngas. This section describes the different types of available reforming technologies.

2.1.1 Steam Reforming

Steam reforming is an industrial process that is used for commercial production of syngas, a mixture of hydrogen and carbon monoxide from carbonaceous species such as natural gas, crude oil and biomass (Muñoz *et al*, 2019). This is achieved in a steam reformer which consists of several hundreds of fixed-bed reactor tubes filled with metal-based catalyst such as nickel on alumina or zeolite (Pandey *et al*, 2015). The flow sheet for steam reforming process is shown on figure 2-1 which was obtained from AL-Megeren and Xiao (2012). The catalyst shapes used in steam reforming process are: spokes with wheels, gear wheels and spoked wheels (Rainer, 2011). The advantage of these shapes is low pressure drop (Rainer, 2011). Steam at high temperature which is 600 – 1100 °C and high pressure 1500 – 3000 kPa reacts with carbonaceous feed material to produce hydrogen and carbon monoxide (Albonetti *et al*, 2019).

Steam reforming is widely used in the production of commercial bulk hydrogen which constitute approximate 95 % of the 70 million tons produced globally (Jens, 2019). Hydrogen is used in the industrial preparation of fertiliser chemicals such as ammonia in the Haber-Bosch process, preparation of hydrogenated vegetable fats such as margarine, energy production from fuel cells etc (Rostrup-Nielsen and Rostrup-Nielsen, 2002). The following equations describes the steam reforming of any oxygenated hydrocarbon and subsequent water gas shift reactions:



At low temperatures, the formation of methane according to the equation below is also possible:



Steam reforming reaction 1 is endothermic and reversible, hence it is favoured by high temperature, low pressure and high steam addition. The optimum operating conditions for steam reforming is highly dependent on the feedstock used, with the larger molecules requiring harsh reaction conditions such as higher temperature for improved conversion. Nonetheless, the highest operating temperature for any feedstock is limited to what the catalyst can withstand in case of catalysed steam reforming (Azinal, 2019).

The water gas shift reaction 2 produces more hydrogen by reaction carbon monoxide from reaction 1 with more steam. This makes the overall process more economical than earlier processes for hydrogen production such as reacting steam with iron (Chandra *et al*, 2009). Furthermore, the water gas shift reaction is moderately exothermic with $-41,2$ kJ/mol heat of reaction (Chandra *et al*, 2009). Therefore, an increase in reaction temperatures shifts the equilibrium towards the reactants making the production of carbon monoxide less favourable (Chandra *et al*, 2009).

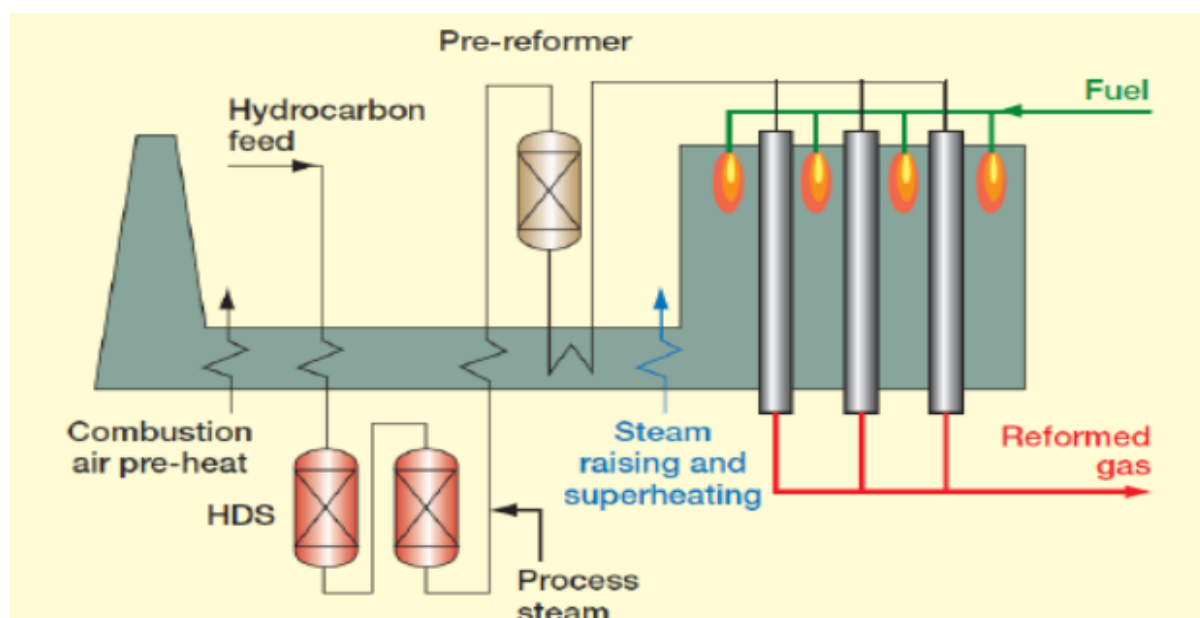


Figure 2-1: Industrial steam reforming process (AL-Megeren and Xiao, 2012)

2.1.2 Dry Reforming

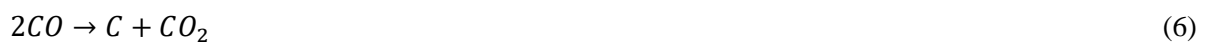
Dry reforming is a type of process used to produce synthesis gas by reacting carbon dioxide with carbonaceous feedstock, traditionally methane. Due to continuous effort to reduce the contribution of the emission of greenhouse gases to global warming, dry reforming has gained increasing interest over alternative reforming technologies such as steam reforming. Dry reforming is mostly suitable when syngas which a high CO content is required (Wang and Economide, 2009). The greenhouse gases consumed during the dry reforming process are carbon dioxide and methane if it used as feedstock. The governing reaction is as follows:



The reaction is carried out at high temperatures, typically 700 – 900 °C and atmospheric pressure (Yang and Ge, 2016). Rhodium and Ruthenium are commonly used dry reforming catalysts since Nickel is easily deactivated by coke formation (Wang and Economide, 2009). Furthermore, Nickel catalyst catalyse carbon deposition according to the reaction:



Carbon can also be deposited via the Boudouard reaction which is:



The H₂/CO ratio of syngas produced by dry reforming process is 1:1 which is preferred for the Fischer–Tropsch synthesis to produce synthetic fuels (Yang and Ge, 2016)

2.1.3 Partial Oxidation

Partial oxidation occurs when a sub-stoichiometric amount of air exothermically reacts with a carbonaceous feedstock (Gunardson and Abrardo, 1999). Due to incomplete combustions during partial

oxidation, hydrogen gas is produced along with carbon monoxide (Speight, 2015). The equation describing partial oxidation of any oxygenated hydro-carbonaceous feed is presented below:



Partial oxidation occurs in two stages. In the first stage, carbonaceous feedstock is converted to CO₂ and H₂O until O₂ is completely consumed (Kalai, 2015). In the second stage, syngas is produced via Dry Reforming and Steam Reforming Reactions 4 and 1, respectively (Kalai, 2015).

The heat released from the exothermic partial oxidation is used to heat the reaction chamber to the region of 870 °C (Speight, 2015). The advantage of partial oxidation is that it can be used for almost any carbonaceous feedstock which includes heavy petroleum residues (Speight, 2015). Furthermore, partial oxidation is environmental benign since the emission of environmentally degrading oxides of Nitrogen and Sulfur, (NO_x) and (SO_x) is reduced (Speight, 2015).

As outlined by Kalai (2015) there are numerous advantages of partial oxidation over steam reforming. These advantages are outlined below:

- Partial oxidation reactor is cheaper to construct due to the partial oxidation reaction being mildly exothermic compared to the highly exothermic steam reforming reactions. Furthermore, partial oxidation can be combined with endothermic reactions during steam reforming or dry methane reforming to maximise energy recovery thereby making the process more energy efficient.
- Stoichiometric fed partial oxidation produces syngas with H₂/CO ratio of 2. Syngas with this ratio is suitable for methanol production as well as production of liquid fuels via the Fischer-Tropsch synthesis. This eliminates the need for correcting the syngas H₂/CO ratio which is usually high in the steam reforming process.
- Syngas produced by partial oxidation has low content of CO₂ which often has to be removed. This leads to more economical use of syngas.
- Partial oxidation does not require steam usage which keeps the process more economical due to avoidance of high production and distribution cost of steam.

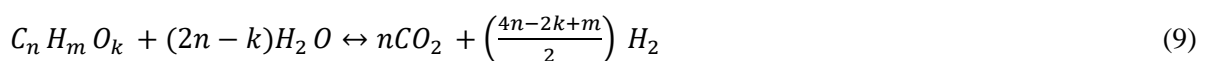
2.1.4 Aqueous Phase Reforming

Aqueous phase reforming produces hydrogen gas based, mainly, on biomass derived hydrogenated feedstocks such as glycerol, sugars, and sugar alcohols (Bhaskar *et al*, 2013). This reaction takes place in excess liquid (Azizan, 2014). Furthermore, there is no water volatilization required which results in higher energy efficiency compared to other reforming processes (Bhaskar *et al*, 2013). Aqueous phase reforming is carried out at low temperatures below 200 - 250 °C and high pressure between 15 – 50 bar (Wilson, 2014) (Bhaskar *et al*, 2013). At low temperature and high pressure, the water gas shift reaction shown below favours the production of hydrogen gas rich syngas without having to use multiple reactors as done in steam reforming (Davda and Dumesic, 2003).



Moreover, carrying out the reaction at low temperatures prevents unwanted decomposition which is notable when the feedstock is heated (Bhaskar *et al*, 2013).

The reaction route for aqueous phase reforming process involves the cleavage of C-C, C-H and O-H bond to form adsorbed species on the catalyst surface (Manfro *et al*, 2011). The cleavage of C-C bond produces CO after which the water gas shift reaction takes place over the supported catalyst (Azizan, 2014). Fixed bed or high throughput reactor is suitable for aqueous phase reforming. The overall reaction for hydrogen gas production by aqueous phase reforming is shown below:

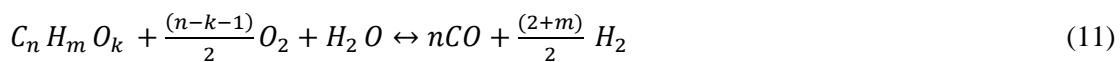
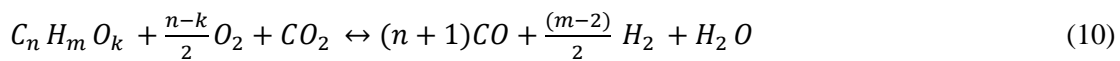


2.1.5 Autothermal Reforming

In this process, the partial oxidation reaction which is exothermic supplies heat to the steam reforming process which is endothermic (Brett, 2012). In this process the feedstock, steam, carbon dioxide are mixed directly with air in the reforming unit (Speight, 2014). Autothermal reforming is popular among small scale hydrogen production plants with an advantage of producing higher hydrogen yield than partial oxidation and quicker start-up and reaction time than steam reforming (Brett, 2012). Effective

heat management is achieved by independent control of steam to carbon and air to fuel ratios, respectively (Brett, 2012).

The autothermal reformer is comprised of three zones: The burner where all streams fed are turbulently mixed in a diffusion flame, the combustions zone where partial oxidation reactions takes places to produce hydrogen and carbon monoxide mixture, and the catalytic zone where the gases exiting the combustion zone reach thermodynamic equilibrium (Speight, 2015). Partial oxidation takes places in the combustion zone and the mixture formed flows through a bed of catalyst at which the reaction takes place (Speight, 2015). The reactions for autothermal reaction using carbon dioxide and steam, respectively are shown below:



In the case of methane autothermal reforming, when carbon monoxide is used the syngas gas produced has a H₂/CO ratio of 1 compared to 2,5 in the case of steam (Speight, 2014). The advantages of autothermal reforming are: compact design, low initial capital cost, lower operating cost for larger plants, flexible operation and soot free operation (Speight, 2014).

2.1.6 Tri Reforming

Tri reforming is a synergetic combination of steam reforming, dry reforming and partial oxidation reactions, 1, 4 and 7, respectively (Jilani and Kumar, 2020). Flue gas components from fossil-based power plants which are H₂O, CO₂ and O₂ are used as co-reactants for tri-reforming process to produce syngas (Jilani and Kumar, 2020). De Campos Roseno (2017) produced a process flowsheet for tri reforming process which is shown on figure 2-2. Tri reforming process has been designed to produce syngas with the desired H₂/CO ratio by using flue gas from fossil-based power plant without having to separate CO₂ from the flue gas (Jilani and Kumar, 2020).

The two important missions that are achieved by combining steam reforming with dry reforming are production of a desired H₂/CO ratio and mitigating carbon deposition that is problematic for dry reforming (Song and Pan ,2004). Integrating steam reforming and partial oxidation with dry reforming can reduce catalyst poisoning by carbon deposition which will increase catalyst life and overall process efficiency. Therefore, tri reforming solves problems which are entered by individual reforming processes.

Two of the most common uses of syngas are methanol production and Fischer-Tropsch synthesis which accounts for 19 % of the global syngas market according to El-Nagar and Ghanem (2019) requires H₂/CO ratio of 2. Syngas from steam reforming process has high H₂/CO ratio around 3, while from dry reforming process syngas has a lower H₂/CO ratio of < 1 therefore, syngas from these two processes requires further treatment to adjust the H₂/CO ratio. Even though partial oxidation produces syngas with H₂/CO ratio of 2, it is difficult to control due to exothermic nature of the reactions and expensive to operate due to requirement of pure O₂ as opposed to air. For this reason, tri reforming is the preferred process since it can produce syngas with H₂/CO ratio of 1,5 – 2 under mild conditions.

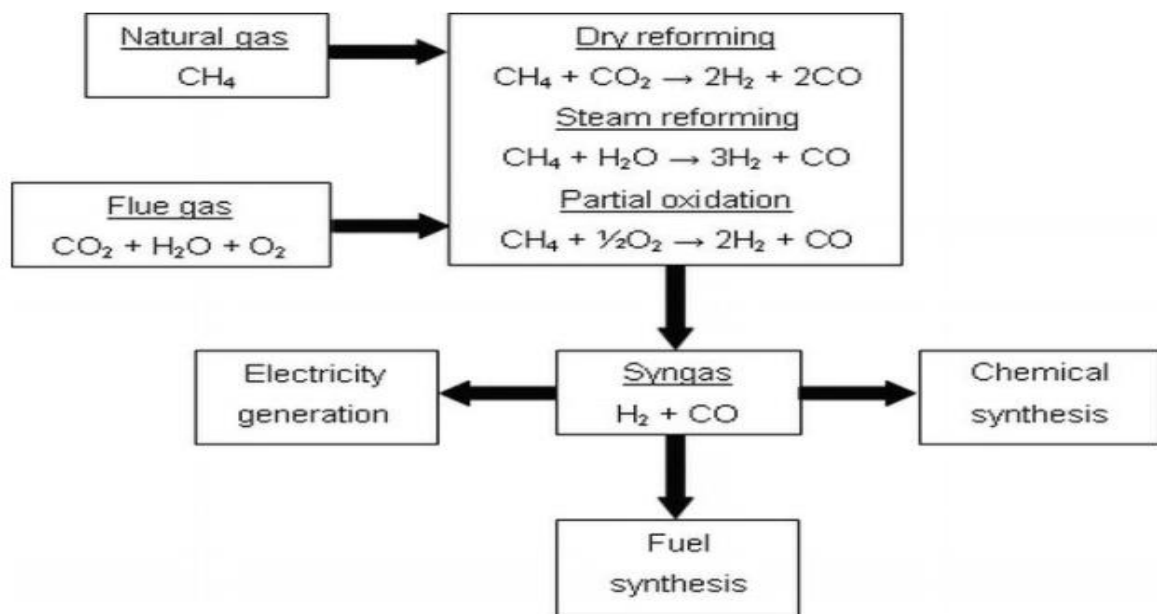


Figure 2-2: Tri reforming process flow flowsheet for natural gas (De Campos Roseno, 2017)

2.2 Feedstocks for Syngas Production via Steam Reforming Process

2.2.1 Traditional Feedstocks: Non-Renewable

Since its development in the early 1900's, steam reforming process has been carried out using fossil fuel-based feedstocks such as oil, coal, and gas (Murkin and Brightling, 2016). Fossil fuels forms when a large quantity of dead plant and animal matter is buried below the surface of the earth is exposed to high heat and pressure over time (Mann, 2003). Fossil fuels cannot replenish at the same rate as they are consumed, hence the supply chain is threatened due to the depletion of its reserves (Mann, 2003). Moreover, fossil fuel usage leads to an increase in global warming because of greenhouse gas emission.

2.2.1.1 Natural Gas – Methane

Natural gas is a natural occurring mixture of hydrocarbon gases that consist mainly of methane (Natural Gas Supply Association, 2014). Natural gas also includes higher alkanes, carbon dioxide, nitrogen, hydrogen sulfide and helium (Natural Gas Supply Association, 2014). The composition of a typical natural gas is shown on table 2-1. Natural gas is the most important and widely used feedstock for steam reforming mainly due to its availability, ease of handling, high hydrogen to carbon ratio (National Research Council, 2004).

Table 2-1: Typical composition of natural gas (Natural Gas Supply Association, 2014)

Name of Compound	Chemical Formulae	Composition
Methane	CH ₄	70 – 90 %
Ethane	C ₂ H ₆	0 – 20 %
Propane	C ₃ H ₈	
Butane	C ₄ H ₁₀	
Carbon Dioxide	CO ₂	0 – 8 %
Oxygen	O ₂	0 – 0.2 %
Nitrogen	N ₂	0 – 5 %
Hydrogen Sulfide	H ₂ S	0 – 5 %
Rare Gases	Ar, He, Ne, Xe	Trace

The reaction for steam reforming of methane is:



Due to high H₂/CO ratio, steam methane reforming is ideal for producing high purity hydrogen (Neiva and Gama, 2010). Steam methane reforming is a mature process which makes it a good starting point for transition to a hydrogen economy, however, syngas produced from methane steam reforming is still expensive for hydrogen cost targets in the petroleum industry (Neiva and Gama, 2010).

2.2.1.2 Coal

Coal is a black or brownish black combustible sedimentary rock that is found on the earth's surface (Blander, 2011). It is comprised mainly of carbon and a variable amount of other components which are: hydrogen, sulfur, nitrogen and oxygen (Blander, 2011). Coal is best known and widely used for electricity generation in coal fired power stations worldwide (World Coal Association, 2015). The drawback of coal combustion in coal fired power stations is the emission of greenhouse gases (World Coal Association, 2015).

An alternative to coal combustion is coal gasification which produces syngas that can be used to generate electricity using reciprocating engines, gas turbines or fuel cell with greater electrical efficiency than steam turbines used in coal fired power station (Roos, 2010). Moreover, gasification allows an Integrated Gasification Combined Cycle (IGCC) which is an efficient process for generation of electricity at higher efficiency to be used (Roos, 2010). During the Integrated Gasification Combined Cycle (IGCC), syngas is burnt in a gas turbine to generate electricity (Roos, 2010). Waste heat from both the gasifier and steam turbine is recovered in a waste heat boiler to generate steam which in turn is used to produce electricity in a steam turbine (Roos, 2010).

2.2.1.3 Crude Oil/Residues

Crude oil which is commonly referred to as oil is a natural occurring yellowish-black liquid fuel made up of a mixture of hydrocarbons drilled beneath the earth's surface. The hydrocarbons present in crude oil are predominantly alkanes, naphthenes, aromatics and asphaltic. The typical relative portion of hydrocarbons present on crude oil is shown in table 2-2. In additions to a mixture of hydrocarbons, crude oil is comprised of nitrogen, sulfur and oxygen.

Many refiners are constantly on the lookout for means to maximise yield of high value products from different grades of crude oil (Wolff and Vliegthart, 2011). Gasification offers an opportunity for alternative treatment of petroleum products such as heavy oil residues which has been treated by burning as a fuel. Gasification of heavy oil residues is particularly important as the restrictions on sulphur dioxide emission from the combustion of fuels is increasingly becoming stricter (Navarro et al, 2010). Moreover, heavy oil residues gasification can be used for production of hydrogen which is used in the hydrocracker unit in the refinery (Navarro et al, 2010)

Table 2-2: Different types of hydrocarbons that appears in crude oil (Hyne, 2001)

Hydrocarbon	Average Composition (wt %)	Composition Range (wt %)
Alkanes (Paraffins)	30 %	15 – 60 %
Naphthenes	49 %	30 – 60 %
Aromatics	15 %	3 -30 %
Asphaltics	6 %	Remainder

2.2.2 Alternative Feedstocks: Renewable

2.2.2.1 Biomass

Driven by the growing interest in bioenergy, biomass utilisation has gained wide interest as an alternative to fossil fuels (Balat and Kirtay, 2010). The sources of biomass are wood, agricultural crops, municipal solid waste, animal wastes, food waste, and aquatic plants and algae (Balat and kirtay, 2010). Biomass steam reforming (and other thermochemical processes) is preferred over biological conversion due to high overall thermal efficiency and lower production cost (Balat and kirtay, 2010).

2.2.2.2 Waste Plastics

As a result of increasing industrial and consumer demand in line with an increase in world's population, the volume of plastic waste generated is on the rise. Even though waste plastics can be re-used and recycled, an effective solution to the problems posed by waste plastics is required. The reason for this is that waste plastics can only be re-used a finite number of times which means that, at the end waste plastics becomes garbage.

Amongst others, the dominant type of plastics produced are polyethylene and polypropylene (Saad and Williams, 2016). Polyethylene makes up 29,6 % of plastics produced while polypropylene makes up 18,9 % (Saad and Williams, 2016). To increase the value of waste plastics, technologies such as steam reforming has received increasing attention due to their high hydrocarbon content. Many researchers have studied the thermochemical conversion of waste plastics to produce H₂ and syngas (Saad and Williams, 2016).

2.2.2.3 Waste Tyres

A large volume of waste tyres is produced worldwide. Waste tyres has been treated through energy recovery such as waste derived fuels and material recycle (Zhang et al, 2016). Waste tyres is comprised mainly of elastomers such as natural rubber, butadiene and styrene-butadiene rubbers as well as carbon black filler and other additives (Zhang et al, 2016). The typical composition of waste tyre 81,2 wt % carbon and 7,2 wt % hydrogen (Zhang et al, 2016). Moreover, waste tyres have high volatiles, low ash content and higher heating value than materials such as coal and biomass, hence it is an excellent feedstock for steam reforming process (Portofino et al, 2011). Pyrolysis of waste tyres has been studied by many researchers (Williams, 2013).

2.2.2.4 Other Feedstocks

Other feedstocks such as Municipal Solid Waste, Black Liquor, Waste Office Paper, Food Waste etc are also viable for syngas production using thermochemical processes such as steam reforming.

2.3 Analysis of Different Feedstocks

The list of feedstocks selected for this work are Rice Husk, Wood Chips, Sugarcane Bagasse, Food Waste, Municipal Solid Waste (MSW), Waste Office Paper, Waste Plastics (PE), Waste Plastics (PP), Waste Tyres, Coal, Crude Oil (Iraq), Black Liquor (from Alkaline Pulping of Straw), Poultry Manure, Pig Manure, Dairy Manure. The next sections describe the type of feedstock composition used for all feedstock selected for use in simulations.

2.3.1 Composition of Different Feedstocks

Feedstock composition is one the most important information that needs to be known for simulating the steam reforming process on ASPEN Plus. The required composition is obtained from ultimate and proximate analysis of each feedstock. Ultimate analysis commonly referred to as elemental analysis is the method for determining the amount of Carbon, Hydrogen, Nitrogen, Sulfur and Oxygen present in the feedstock. Ultimate analysis is important for understanding the properties of feedstock to evaluate its utility. Proximate analyse determines the Volatile Matter, Ash, Fixed Carbon of a feedstock on dry basis. The ultimate and proximate analysis of feedstocks considered in this work is shown on table 2-3:

Table 2-3: Ultimate analysis of different feedstocks from different sources in the literature

Feedstock	Ultimate Analysis ***							
	C	H	O	N	S	Cl	Ash	Total
Wood Chips (Pröll and Hofbauer, 2008)	51,29	6,09	41,38	0,20	0,02	0,05	0,97	100,00
Sugarcane Bagasse (Hugo, 2010)	47,64	5,92	40,82	0,29	0,07	-	5,26	100,00
Rice Husk (Yao, 2008)	44,62	5,09	33,85	0,47	0,06	-	15,90	100,00
Food Waste (Naveed et al, 2009)	57,87	8,95	24,05	4,04	0,19	-	4,90	100,00
Municipal Solid Waste (Naveed et al, 2009)	39,75	5,43	11,08	1,57	0,88	-	41,29	100,00
Waste Office Paper (Fan et al, 2015)	34,56	4,30	48,25	-	0,09	-	12,80	100,00
Waste Plastics (PE) (Wilk and Hofbauer, 2013)	85,81	13,86	0,00	0,12	0,06	-	0,15	100,00
Waste Plastics (PP) (Xiao, 2007)	86,17	12,24	0,00	0,72	0,17	-	0,70	100,00
Waste Tyres (Osayi et al, 2017)	71,40	4,62	6,80	0,18	1,01	-	16,00	100,00
Crude Oil (Iraq) (Peng et al, 2017)	48,49	7,38	28,50	4,80	-	-	10,83	100,00
Coal (liu et al, 2017)	72,73	5,13	7,86	1,48	2,86	-	9,94	100,00
Black Liquor (Alkaline Pulping of Straw) (Pue'rtolas et al, 2000)	37,09	4,31	35,56	0,95	3,32	-	18,75	100,00
Poultry Manure (Font-Palmer, 2012)	39,14	5,35	33,21	3,87	0,48	1,02	16,93	100,00
Pig Manure (Xiao et al, 2012)	36,64	4,92	38,09	4,54	0,88	0,00	14,92	100,00
Dairy Manure (Fernandez- Lopez et al, 2017)	40,74	5,32	31,36	1,38	0,41	-	20,78	100,00

*** Data from original reference that did not add up to 100 % was normalised to equate the sum of individual analysis to 100 %

Table 2-4: Proximate Analysis of different feedstocks from different sources in the literature

Feedstock	Proximate Analysis ***					HHV
	Total	Moisture	Fixed Carbon	Volatile Matter	Ash	MJ/kg
Wood Chips (Pröll and Hofbauer, 2008)	100,00	16,67	15,70	66,67	0,97	19,09
Sugarcane Bagasse (Hugo, 2010)	100,00	6,37	11,14	77,25	5,24	18,70
Rice Husk (Yao, 2008)	100,00	12,81	13,91	57,36	15,92	14,28
Food Waste (Naveed <i>et al</i> , 2009)	100,00	29,33	14,61	51,15	4,90	26,53
Municipal Solid Waste (Naveed <i>et al</i> , 2009)	100,00	10,71	13,81	34,19	41,29	18,00
Waste Office Paper (Fan <i>et al</i> , 2015)	100,00	4,50	10,80	71,90	12,80	11,11
Waste Plastics (PE) (Wilk and Hofbauer, 2013)	100,00	0,02	0,00	99,83	0,15	43,99
Waste Plastics (PP) (Xiao, 2007)	100,00	0,00	0,00	99,30	0,70	44,70
Waste Tyres (Osayi <i>et al</i> , 2017)	100,00	0,50	27,10	56,40	16,00	31,22
Crude Oil (Iraq) (Peng <i>et al</i> , 2017)	100,00	9,12	12,03	68,02	10,83	23,79
Coal (liu <i>et al</i> , 2017)	100,00	10,20	44,65	35,35	9,80	27,13
Black Liquor (Alkaline Pulping of Straw) (Pue'rtolas <i>et al</i> , 2000)	100,00	9,09	12,17	59,98	18,75	14,18
Poultry Manure (Font-Palmer, 2012)	100,00	21,51	10,57	51,00	16,93	14,79
Pig Manure (Xiao <i>et al</i> , 2012)	100,00	17,77	13,21	54,09	14,92	14,46
Dairy Manure (Fernandez-Lopez <i>et al</i> , 2017)	100,00	3,45	11,68	64,09	20,78	18,40

*** Data from original reference that did not add up to 100 % was normalised to equate the sum of individual analysis to 100 %

2.3.2 Thermodynamic Analysis of Steam Reforming Process

Steam reforming is a thermochemical process, hence accurate thermodynamic data is necessary for process design, analysis, and optimisation. The parameters described are feedstock heating value, syngas heating value and cold gasification efficiency.

2.3.2.1 Heating Value of Solid Fuel

Heating value is the quantity of heat that is produced when a unit mass of a substance has combusted completely at standard conditions which is 25 °C and 1 atm (Sun, 2009). Heating value is dependent on the phase of water present when the substance has combusted. When the water is present in gas phase, the heating value is called Lower Heating Value (LHV). When the water is present in the liquid phase, the heating value is called Higher Heating Value (HHV). The difference between the lower heating value and the higher heating value is the latent heat of vaporisation.

Heating values can be determined experimentally or from correlations using the ultimate and proximate analysis (Demirbas, 1996). Experimental determination of heating value requires specialised equipment whereas ultimate and proximate analysis is obtained from common laboratory equipment (Bushnell *et al*, 1989). Demirbas (1996) developed a formulae for determination of HHV of biomass fuels from proximate analysis and is reported below:

$$HHV = 0,312FC + 0,1534VM \quad (13)$$

Where HHV is the Higher Heating Value of the feedstock in MJ/kg, FC is Fixed Carbon in wt % and VM is Volatile Matter in wt %. Since the heat released by a substance is dependent on the recombination of elements that makes up the fuel, the most accurate estimate for the heating value is obtained from elemental analysis of the fuel (Hosokai *et al*, 2016). The modified version of the Dulong's equation has been proven to reliably predict heating value of a wide range of gas, liquid, and solid fuels with mean absolute error of 2,6 % (Hosokai *et al*, 2016). The modified Dulong's equation as presented by Hosokai *et al* (2016) is shown below:

$$LHV = 32,8C + 84,9\left(H - \frac{O}{8}\right) - (0,15 + 0,12) \quad (14)$$

Where LHV is the Lower Heating Value of the fuel in MJ/kg, C, H and O are wt% of Carbon, Hydrogen and Oxygen, respectively, of the fuel from its elemental analysis on dry ash free basis.

2.3.2.2 Lower Heating Value of Syngas

For syngas, LHV is one of the most important parameters, particularly when syngas is used for energy applications such as in CHP where heat and energy is generated by syngas using fuel cells or other technologies. Syngas LHV is the mole fraction weighted sum of LHV of individual combustible substances found in the syngas which are predominantly: CO, H₂ and CH₄. Moghadam *et al* (2014) reported the following equation for syngas LHV calculation:

$$LHV = \frac{126,36CO + 107,98H_2 + 358,18CH_4}{1000} \quad (14)$$

Where LHV is the Lower Heating Value in MJ/Nm³ and CO, H₂ and CH₄ are dry basis mole fraction of Carbon Monoxide, Hydrogen and Methane in syngas, respectively.

2.3.2.3 Cold Gasification Efficiency (CGE)

In order to determine the actual technical operation and economic feasibility of a gasifier system, an important parameter to measure is the cold gasification efficiency. Cold gasification efficiency is defined by Gai and Dong (2011) as the ratio of the lower heating value of cold syngas to the higher heating value of the feedstock/fuel. Demirbas (1996) provided the following equation for calculating the gasifier CGE:

$$CGE = \frac{G_p \times LHV_{\text{syngas}}}{HHV_{\text{fuel}}} \quad (15)$$

Where G_p is the syngas yield which is the ratio of syngas volumetric flow to the quantity of feedstock fed and is expressed in Nm³/kg, LHV_{syngas} is the lower heating value of syngas in MJ/Nm³ and HHV_{fuel} is the higher heating value of the feedstock/fuel in MJ/kg.

2.4 Uses of Syngas

El-Nagar and Ghanem (2019) mentioned that the global syngas market is comprised of: Ammonia, Hydrogen, Methanol, Gas to Liquid, Electricity and Other. The percentage proportion of each use in the globally share is shown on figure 2-3.

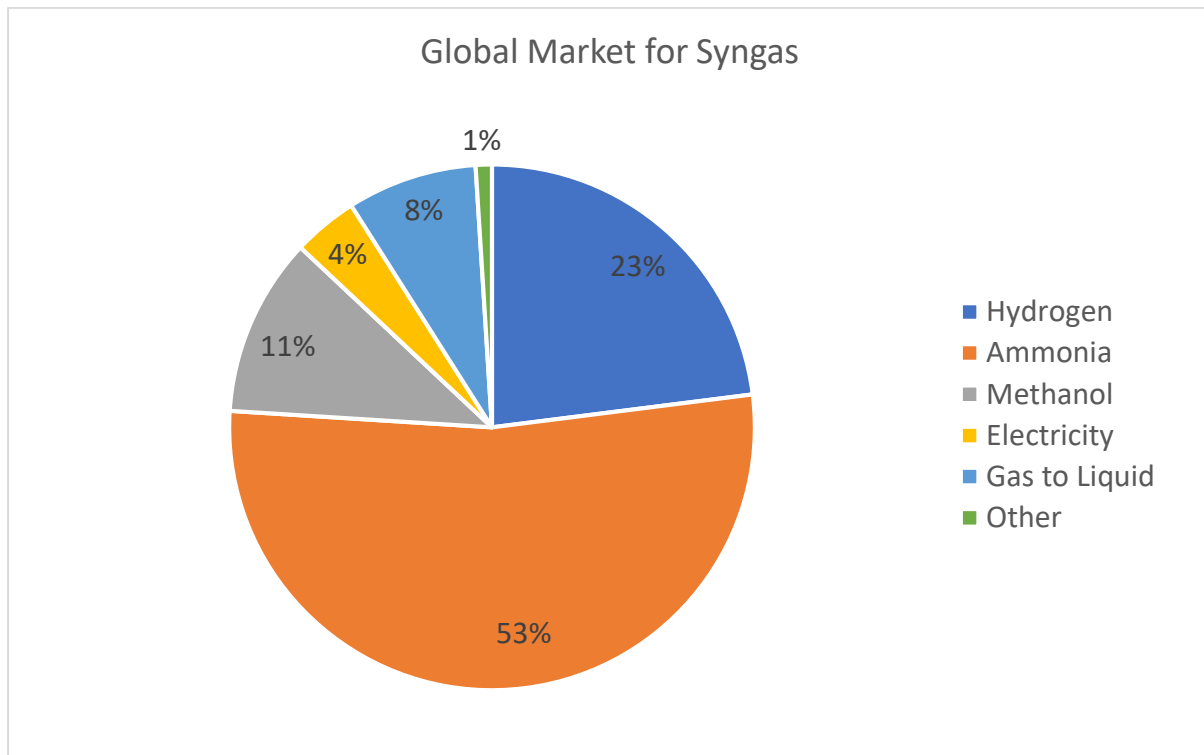


Figure 2-3: Global syngas market (El-Nagar and Ghanem, 2019)

Syngas as a chemical intermediate is used in the chemical industry for synthesis of a wide variety of chemicals. Figure 2-4 show some of the chemicals that are produced from syngas as feedstock (Sharma, 2018)

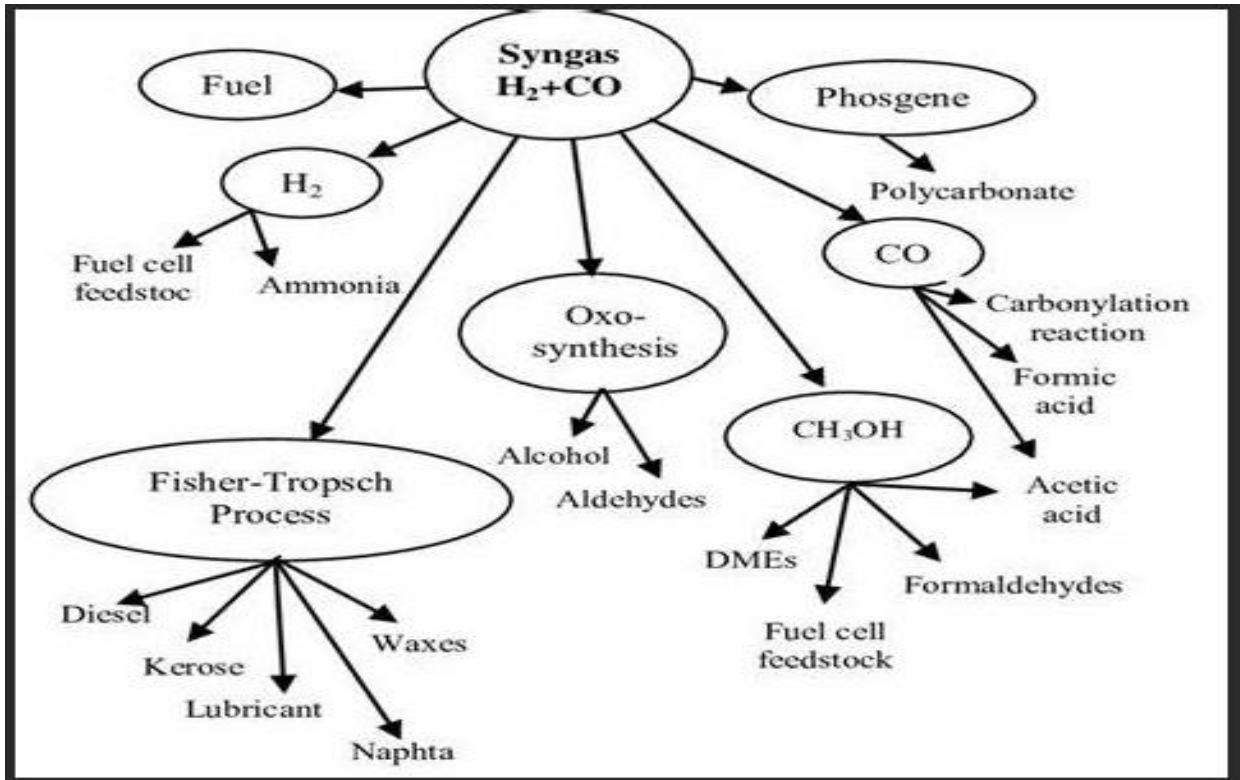


Figure 2-4: Wide variety of chemical that can be produced from syngas (Sharma, 2018)

2.4.1 Ammonia

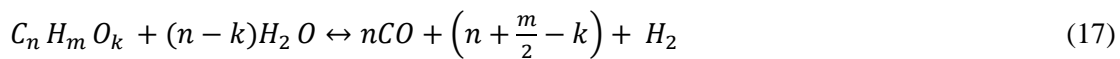
As indicated on figure 2-3, 53 % of syngas produced globally is used in the production of Ammonia (El-Nagar and Ghanem, 2019). Ammonia is a compound of hydrogen and nitrogen and its molecular formulae is NH_3 . The main uses for ammonia is in the production of nitrogen based fertilisers (El-Moneim *et al*, 2018). The hydrogen used in the production of ammonia is obtained from steam reforming process whereas nitrogen is obtained from atmospheric air (El-Moneim *et al*, 2018). The widely used process for the industrial production of ammonia is the Haber-Bosch process (El-Moneim *et al*, 2018). The reaction for production of Ammonia is:



2.4.2 Hydrogen

Syngas can be cleaned via separation processes such as pressure swing adsorption or amine adsorption to produce high purity hydrogen. Pressure swing adsorption is the most common hydrogen purification process. During purification, syngas enters the purifier, where specific absorptive materials trap contaminants such as carbon dioxide, methane, carbon monoxide, and water from hydrogen at high pressures. High purity hydrogen is then pumped out of the vessel after which the vessel is de-pressurized to release the trapped contaminants.

Hydrogen is used in the industrial preparation of fertiliser chemicals such as ammonia in the Haber-Bosch process, preparation of hydrogenated vegetable fats such as margarine and energy production from fuel cells etc. (Rostrup-Nielsen, 1998). The following equations describes the steam reforming of any oxygenated hydrocarbon and water gas shift reactions used in the production of hydrogen:



2.4.3 Methanol

Methanol is amongst the most important feedstocks used in the chemical industry (Lucking, 2017). Amongst others, it uses include use as a solvent, anti-freeze, and windshield wiper fluid (Olsbye *et al*, 2012). Methanol is the product of low pressure catalytic reaction of syngas (Lucking, 2017). The reactions to produce methanol are shown below:



2.4.4 Gas to Liquid

Syngas can also be converted to liquid hydrocarbons such as lubricating oil and synthetic fuel via a series of chemical reactions known as the Fischer-Tropsch (de Klerk, 2013). The important reaction during the Fischer-Tropsch series is the production of alkanes with the formula C_nH_{2n+2} , the reaction is:



Where n is usually between 10 and 20. Most alkanes produced during these reactions are usually straight chained which makes the fuel produced suitable for use as diesel fuel. Even though alkanes are the main products, competing reactions leads to the formation of alkenes, alcohol, and other hydrocarbons (Takao, 2001).

2.4.5 Electricity Generation

Syngas can also be utilised for electricity generation using technologies such as gas turbine, reciprocating engine, and fuel cell (Roos, 2010). Syngas fuelled engines has higher electrical efficiency compared to steam turbine, particularly when integrated combined cycle is used (Roos, 2010). The requirement for syngas to be used for electricity generation is that it should be clean and free from tar and particulate matter (Roos, 2010)

2.5 Introduction to ASPEN Plus

ASPEN Plus is a leading chemical process simulator in the field of chemical engineering. ASPEN Plus allows the user to build process model and simulate them using complex mass & energy balance and equilibrium calculations. It originated in the 1970's from a joint venture project called **A**dvanced **S**ystem for **P**rocess **E**ngineering (ASPEN) between Massachusetts Institute of Technology (MIT) and the US Department of Energy (Sun, 2009). ASPEN Plus is a product of ASPEN Technology Inc which is a software and services company headquartered in Bedford, Massachusetts and listed on the NASDAQ stock exchange (ASPEN Technology Inc, 2013).

ASPEN Plus is widely used in chemical industry and engineering education institutions in research, development, design, and modelling of chemical processes. It provides a comprehensive data base for physical property and unit operations model (Sun, 2009). Furthermore, ASPEN Plus offers a fast and reliable functions and calculation methods to save time and eliminate human error in execution of complex chemical engineering calculations models. ASPEN Plus has been used by many researchers for modelling and simulation of steam reforming processes. ASPEN Technology Inc (2013) has provided detailed guidelines for modelling and simulation of chemical processes involving solid materials.

2.5.1 ASPEN Plus Modelling of Steam Reforming Process

For best results, commercial plants require operating variables to be set at or near optimal levels (Sun, 2019). Obtaining optimal values for operating variables from experiments is both expensive and time consuming (Sun, 2019). Even though the results from the model are not always achieved in a real plants, a robust model has the potential to provide a detailed understanding into the effect of changing operating variables on the overall process efficiency and thus allow optimal values for operating variables to be derived (Sun, 2019). To simulate the steam reforming process thermodynamic equilibrium model is often used as opposed to kinetic model (Basu, 2013).

2.5.1.1 Thermodynamic Equilibrium Model

The idea behind the use of equilibrium models is that the maximum possible conversion occurs when the system reaches equilibrium. In equilibrium models, the reaction kinetics are considered unimportant. Furthermore, reactor hydrodynamics are not considered. Moreover, the reactions are considered zero-dimensional and time independent.

For processes such as steam reforming of different heterogeneous waste materials which involves a set of complex chemical reactions, the stoichiometry of the reactions is not considered since all reactions need to be accounted for in the model. Once the reacting system reaches equilibrium, its Gibbs free energy reaches a minimum. This allows the mathematical equation for Gibbs free energy of the system to be minimised subject to the constraints of elemental balance which is obtainable from the ultimate analysis of the feedstock. This approach is particularly useful for feedstocks whose exact composition is unknown such as biomass and different waste materials.

Chapter 3 Methodology

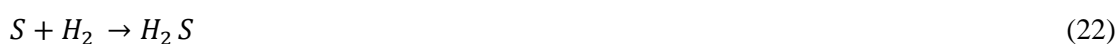
3.1 Simulation of Steam Reforming of Different Feedstocks on ASPEN Plus

This section provides a comprehensive description of the model used on ASPEN Plus V11 to simulate the steam reforming process. The details described are process description, components specification, physical properties, stream specification, block specification and calculator blocks.

3.1.1 Process Description

ASPEN Plus does not have a ready to use reforming model, therefore in order to simulate steam reforming the process is broken down to separate unit operations which can be simulated by an existing model on ASPEN Plus. The models are: 1. Decomposition of feedstock 2. Separation of char and ash 3. Char combustion 4. Reforming/Gasification. Steam reforming, particularly of biomass has been studied extensively by many researchers, as a result the model on ASPEN Plus has been developed by He *et al* (2012), Doherty *et al* (2013), Haugen *et al* (2015), Fernandez-Lopez *et al* (2017) and Ighalo & Adeniyi (2019). The flow sheet for the process to be modelled on ASPEN Plus is shown on figure 3-1.

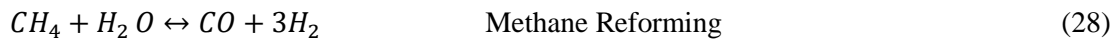
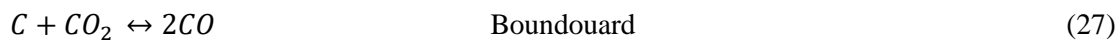
The feed material 'FEEDSTCK' is fed to the RYIELD reactor 'DECOMPOS' which simulates the decomposition to elemental constituents by specifying the yield distribution of each element according to its proximate and ultimate analysis. The outlet 'TOCHARSEP' is comprised of feed elements which are C, H₂, N₂, O₂, S, Cl₂, H₂O, and Ash. 'CHARSEP' separates a portion of char and all ash from the rest of the components. The char and ash are feed to 'COMBUST' which is a RSTOIC block that simulates combustion. The char split fraction is varied by using design specification until the specified gasification temperature is achieved. The stream 'COMBAIR' supplies excess combustion air to 'COMBUST'. The rest of the elements from 'CHARSEP' are feed to 'NONEQUIL' which is a RSTOIC reactor block that simulates the following reactions:





The heat generated from the reactions above is supplied to “GASIF1”. Furthermore, the heat generated by exothermic reaction on ‘COMBUST’ is supplied to ‘GASIF1’ for endothermic reforming reaction. The separator block “GASSEP” removes H₂S, HCl and NH₃ from the outlet stream ‘TOGASSEP’ and the rest of the components are fed ‘GASIF1’ which is an RGIBBS reactor that simulates equilibrium reaction by minimising the Gibbs energy of the system. Steam is also fed to this block for reforming.

The reactions on the reforming unit are:



The outlet stream from ‘GASIF1’ is fed to ‘GASIF2’ where N₂ gas is introduced for purging. The gases H₂S, HCl and NH₃ are heated by ‘GASHEAT’ which is a heater and mixed with the reforming products from ‘GASIF2’ on ‘GASMIX’. ‘IMPSEP’ removes impurities and water from the reforming products to yield only dry synthesis gas.

The following assumptions were made in developing the model:

- The systems is isothermal and at steady state
- Zero dimensional

were chosen to estimate enthalpy of formation, specific heat capacity and density. The proximate and ultimate analysis Wood Chips feedstock is shown on figure 3-1 below:

Table 3-1: Proximate, Ultimate and Sulphur Analysis of feedstock, in this case wood chips biomass

Proximate Analysis		Ultimate Analysis		Sulphur Analysis	
Element	Value (% wt.)	Element	Value (% wt. dry basis)	Element	Value (% wt.)
Moisture (wet basis)	16,67	C	51,29	Organic	0,02
Fixed Carbon (dry basis)	15,70	H ₂	6,09	Pyritic	-
Volatile Matter (dry basis)	66,67	O ₂	41,38	Sulphate	-
Ash (dry basis)	0,97	N ₂	0,20		
		Cl ₂	0,05		
		S	0,02		
		Ash	0,97		

Component ID	Type	Component name	Alias
FEEDSTCK	Nonconventional		
ASH	Nonconventional		
C	Solid	CARBON-GRAPHITE	C
H2	Conventional	HYDROGEN	H2
N2	Conventional	NITROGEN	N2
O2	Conventional	OXYGEN	O2
S	Conventional	SULFUR	S
CL2	Conventional	CHLORINE	CL2
H2O	Conventional	WATER	H2O
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
CH4	Conventional	METHANE	CH4
H2S	Conventional	HYDROGEN-SULFIDE	H2S
NH3	Conventional	AMMONIA	H3N
HCL	Conventional	HYDROGEN-CHLORIDE	HCL

Figure 3-2: Component specification on ASPEN Plus

3.1.3 Physical Properties

PK-MB was selected as the global property method. This method uses the Peng Robinson equation of state modified with Boston Mathias alpha function for all equilibrium properties. The property method input on ASPEN Plus is shown on figure 3-3 below. The stream class for global was specified as “MIXCINC” where “MIX” stand for mixed stream, “CI” conventional inert solids and “NC” non-conventional solids stream. In this simulation, conventional solid is carbon and non-conventional solids are feedstock and ash, respectively.

Property methods & options

Method filter: COMMON

Base method: PR-BM

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

Use true components

Method name: PR-BM [Methods Assistant...]

Modify

EOS: ESPR

Data set: 1

Liquid gamma:

Data set:

Liquid molar enthalpy: HLMX04

Liquid molar volume: VLMX04

Heat of mixing

Poynting correction

Use liquid reference state enthalpy

Figure 3-3: Global Property Method Selection

3.1.4 Stream Specification

The streams were specified according to the table below:

Table 3-2: Stream specification

Stream	Component	Temperature	Pressure	Mass flow rate
FEEDSTCK	Specified as ultimate, proximate and sulphur analysis	25 °C	1 bar	1508,64 kg/hr
COMBAIR	79 vol % Nitrogen 21 vol % Oxygen	450 °C	1 bar	Air to Feed ratio of 1,12
STEAM	100 % Water	450 °C	1 bar	Steam to feed ratio of 0,6
NITROGEN	100 % Nitrogen	25 °C	1 bar	1.372 kg/hr

3.1.5 Block Specification

The block specifications are shown on the table below:

Table 3-3: Block Specification

Block ID	Temperature	Pressure	Specification
COMPOS	25 °C	1 bar	Components yield were specified according to proximate analysis of feedstocks
CHARSEP			Char split fraction was determined by a design specification to achieve target gasifier temperature
NONEQ	25 °C	1 bar	Reaction 22 – 24 were specified with 100 % conversion for S, N ₂ and Cl ₂
GASSEP			100 % separation for HCl, NH ₃ and H ₂ S
GASIF1	850 °C	1 bar	Restrict chemical equilibrium and temperature approach for reactions 25 -29 All components were considered as possible products

GASHEAT	Temperature was determined by a calculate block to equal GASIF1 temperature		Zero pressure drop
GASIF2	Temperature was determined by a calculator block to equal GASIF1 temperature	1 bar	Possible products were specified. They are H ₂ , CO, CO ₂ , CH ₄ , H ₂ O, N ₂ . Equilibrium for reactions 28 -29 were restricted so that the simulation results match the literature results.
IMPSEP			100 % separation for H ₂ O, HCl, H ₂ S and NH ₃
COMBUST	Temperature was determined by a calculate block to be 55 °C above GASIF1 temperature	1 bar	Reaction were generated by ASPEN Plus with NO ₂ as product
ASHSEP			100 % Ash separation

3.1.6 Calculator Blocks

Calculator blocks were used extensively during the model development on ASPEN Plus. The variables used for each calculator block as well the calculation statement as defined in FONTRANS is outlined in this section.

3.1.6.1 Calculator 1

This calculator block was used to calculate the flow of combustion air. The variables used in this calculator block are shown below:

Table 3-4: Definition of variables used in calculator block 1

Variable Name	Variable Classification	Type	Stream	Sub stream	Variable
FEEDFLOW	Import	Stream-Var	FEEDSTCK	NC	MASS-FLOW
AIRFLOW	Export	Stream-Var	COMBAIR	MIXED	MASS-FLOW

The FONTRANS statement below was entered and executed at the beginning of the simulation:

$$\text{AIRFLOW} = 1,12 * \text{FEEDFLOW}$$

4.1.6.2 Calculator 2

This calculator block was used to calculate the flow of steam. The variables used in this calculator block are shown below:

Table 3-5: Definition of variables used in calculator block 2

Variable Name	Variable Classification	Type	Stream	Sub stream	Variable
FEEDFLOW	Import	Stream-Var	FEEDSTCK	NC	MASS-FLOW
MOIST	Import	Stream-Var	TOCHARSP	MIXED	MASS-FLOW
STEAMFLW	Export	Stream-Var	COMBAIR	MIXED	MASS-FLOW

The FONTRANS statement below was entered and executed at the beginning of the simulation:

$$\text{STEAMFLW} = 0.6 * (\text{FEEDFLOW} - \text{MOIST}) - \text{MOIST}$$

3.1.6.3 Calculator 3

This calculator block was used to calculate the temperature of COMBUST. The variables used in this calculator block are shown below:

Table 3-6: Definition of variables used in calculator block 3

Variable Name	Variable Classification	Type	Stream/Block	sub stream	Variable
TGASIFY	Import	Stream-Var	TOGASIF2	NC	MASS-FLOW
TCOMB	Export	Block-Var	COMBUST		TEMP

The FONTRANS statement below was entered and executed at the beginning of the simulation:

$$TCOMB = TGASIFY + 55 \text{ }^{\circ}\text{C}$$

3.1.6.4 Calculator 4

This calculator block was used to calculate the temperature of the gas heat, GASHEAT. The variables used in this calculator block are shown below:

Table 3-7: Definition of variables used in calculator block 4

Variable Name	Variable Classification	Type	Stream/Block	sub stream	Variable
GASIF2TP	Import	Stream-Var	TOGASMIX	MIXED	MASS-FLOW
HEXTEMP	Export	Block-Var	GASHEAT		TEMP

The FONTRANS statement below was entered and executed at the beginning of the simulation:

$$HEXTEMP = GASIF2TP$$

3.1.6.5 Calculator 5

This calculator block was used to calculate the temperature of the gasifier, GASIF2. The variables used in this calculator block are shown below:

Table 3-8: Definition of variables used in calculator block 5

Variable Name	Variable Classification	Type	Stream/Block	sub stream	Variable
TGASIF1	Import	Stream-Var	TOGASIF2	MIXED	TEMP
TGASIF2	Export	Block-Var	GASIF2		TEMP

The FONTRANS statement below was entered and executed at the beginning of the simulation:

TGASIF2 = TGASIF1

Chapter 4 Results

4.1 Model Validation

To validate the results from the model developed in this work, the syngas composition, LHV and CGE from the model was compared with experimental data for steam reforming of Wood Chips from the literature as reported by Pröll *et al* (2004). The model results slightly under predicted the H₂ and CO composition in the syngas. To match the model result to the experimental data from the literature as reported by Pröll *et al* (2004), the restricted equilibrium approach was applied to calibrate the model. This was done by adjusting the temperature approach to equilibrium for reactions 28 – 29 by -280 °C and -145 °C, respectively. The resulting model after calibration produced results which were in good agreement with experimental data from the literature which validates the model. The comparison between the model results and experimental data from the literature is shown on table 4-1 below:

Table 4-1: Comparison between model results and experimental data from literature (Pröll et al, 2004)

Description	H ₂	CO	CO ₂	CH ₄	N ₂	LHV	CGE
	%	%	%	%	%	MJ/kg	%
Simulation	46,17	21,00	21,19	11,58	0,06	11.,78	78,4
Literature	45,80	21,60	21,20	10,00	1,40	11,30	81,12
Absolute Difference	0,37	-0,60	-0,01	1,58	-1,34	0,48	-2,72
Percentage Difference	0,80	-2,78	-0,02	15,82	-96,00	4,24	-3,35

The model was validated using data for wood chips only, hence its reliability is only guaranteed for steam reforming of wood chips feedstock. For other feedstocks, experimental measurements for proximate, ultimate and sulfanal analysis needs to be undertaken to verify the model for a given feedstock prior to construction of commercial plant.

4.2 Syngas Composition, LHV and H₂/CO Ratio for Different Feedstocks

After validation, the model was used to simulate the steam reforming process for different feedstocks at steam temperature of 450 °C, steam to feed ratio of 0,6 , gasifier temperature of 850 °C , combustion air temperature of 450 °C, and combustion air to feed ratio of 1,12. The results for syngas composition (dry basis), syngas LHV as well as syngas H₂/CO ratio as predicted by the model are shown on table 4-3 below:

Table 4-2: Syngas composition, LHV and H₂/CO ratio for different feedstocks at steam temperature of 450 °C, steam to feed ratio of 0,60 , gasifier temperature of 850 °C , combustion air temperature of 450 °C, and air to feed ratio of 1,12.

Feedstock	H ₂	CO	CO ₂	CH ₄	N ₂	LHV	H ₂ /CO
	%	%	%	%	%	MJ/Nm ³	-
Rice Husk	34,49	11,32	31,06	23,06	0,07	5,15	3,05
Wood Chips	46,17	21,00	21,19	11,58	0,06	11,78	2,20
Sugar Cane Bagasse	56,66	31,28	11,26	0,76	0,04	10,06	1,81
Food Waste	7,21	0,60	33,97	58,13	0,10	21,67	12,06
Municipal Solid Waste	5,28	0,31	33,66	60,64	0,12	22,33	16,99
Waste Office Paper	49,02	34,90	16,01	-	0,07	9,69	1,40
Waste Plastics (PE)	3,54	2,76	20,57	73,08	0,05	26,90	1,28
Waste Plastics (PP)	1,97	5,23	22,18	70,57	0,05	26,15	0,38
Waste Tyres	0,33	20,47	25,84	53,30	0,06	21,71	0,02
Coal	0,60	8,82	34,73	55,78	0,07	21,15	0,07
Crude Oil (Iraq)	17,44	3,42	35,05	44,01	0,08	18,07	5,10
Black Liquor (From alkaline pulping of straw)	55,24	28,95	15,64	0,11	0,06	9,65	1,91
Poultry Manure	39,31	10,10	31,85	18,65	0,09	12,20	3,89
Pig Manure	55,12	26,38	18,32	0,12	0,07	9,28	2,09
Dairy Manure	47,03	19,29	21,43	12,19	0,06	7,51	2,44

From the results presented on table 4-3, the H₂/CO is lowest for Waste Tyres and highest for Municipal Solid Waste. Wood Chips, Sugarcane Bagasse, Black Liquor and Pig Manure produced syngas with H₂/CO ratio of 1,81 – 2,20 which is approximately equal to 2,00. A H₂/CO ratio of 2,00 is suitable for Fischer Tropsch process without adjustment. The H₂/CO ratio of the remaining feedstocks would require adjustment either by forward or reverse shift reaction if the target product is synthetic fuel or

methanol. Based on the results, the feedstock to consider for H₂/CO adjustment are Rice Husk, Poultry Manure and Dairy Manure due to good quality syngas and moderate amount of CH₄.

Food Waste, Municipal Solid Waste, Waste Plastics (PP), Waste Plastics (PE), Waste Tyres and Coal produced syngas with poorest quality as indicated by low H₂ and CO content, respectively. Poor syngas quality is attributed to high moisture content in Food Waste, high ash content in Municipal Solid Waste as inferred from proximate analysis shown on table 2-4. In the case of Waste Plastics (PP) and Waste Plastics (PE) poor syngas quality is believed to be due to low fixed carbon in the proximate analysis as shown on table 2.4. The feedstock with poor syngas quality has high LHV due to the presence of CH₄ in significant quantity which makes them suitable for use in energy applications such as Combined Heat and Power (CHP) and Integrated Gasification Combined Cycle (IGCC) as opposed to chemical production.

4.2 Sensitivity Analysis: Effect of Steam Temperature

Steam temperature was varied from 150 – 1000 °C while all other input variables were held constant. The effect of steam temperature on syngas composition, syngas LHV and CGE for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks was studied. The syngas composition presented is reported on dry, NH₃, H₂S and HCl free basis. The gas components NH₃, H₂S and HCl are removed from the analysis because their content is very low and in practice, they are separated downstream by syngas cleaning. The CGE is based on the LHV of syngas and feedstock.

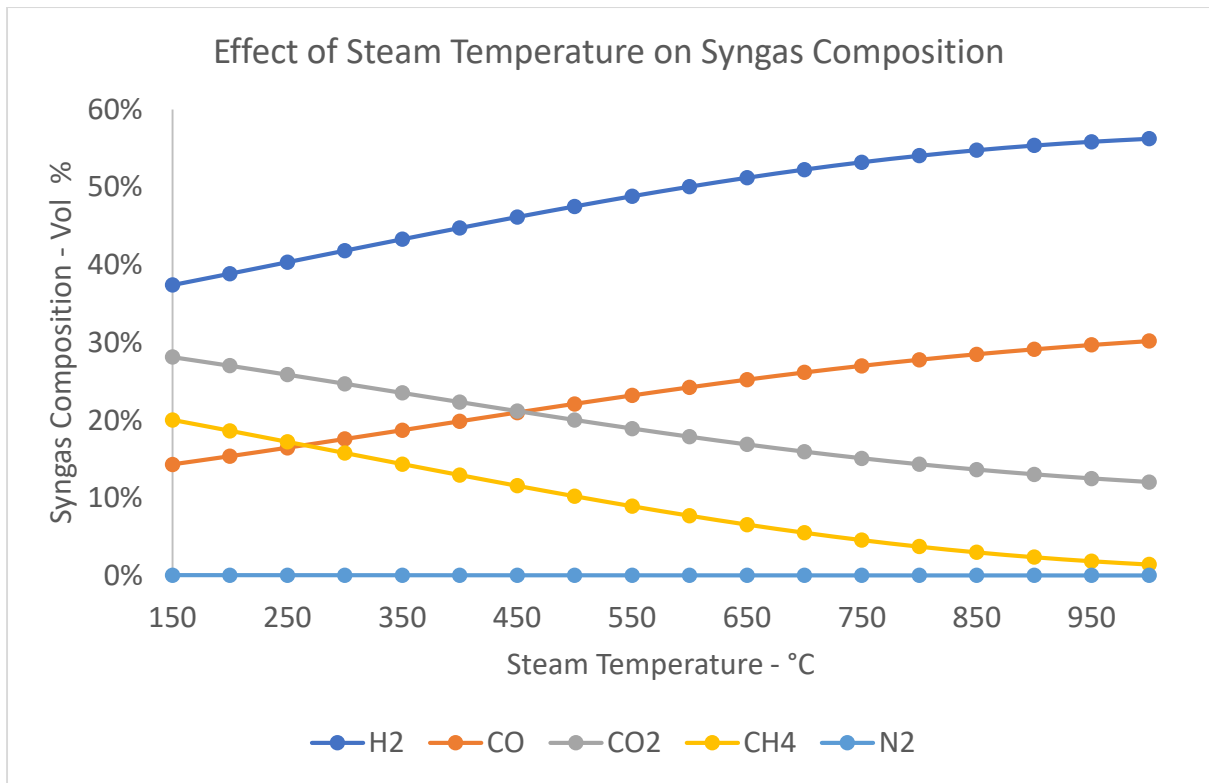


Figure 4-1: Effect of steam temperature on syngas composition for Wood Chips feedstock

As shown on figure 4-1 when the steam temperature is increased from 150 – 1000 °C for Wood Chips feedstock, both H₂ and CO increases. H₂ increase from 37,41 % to 56,25 % while CO increase from 14,33 % to 30,20 %. Contrary to this, both CO₂ and CH₄ drops. CO₂ drops from 28,14 % to 12,06 % and CH₄ drops from 20,05 % to 1,45 %. N₂ also drops from 0,07 % to 0,05 %.

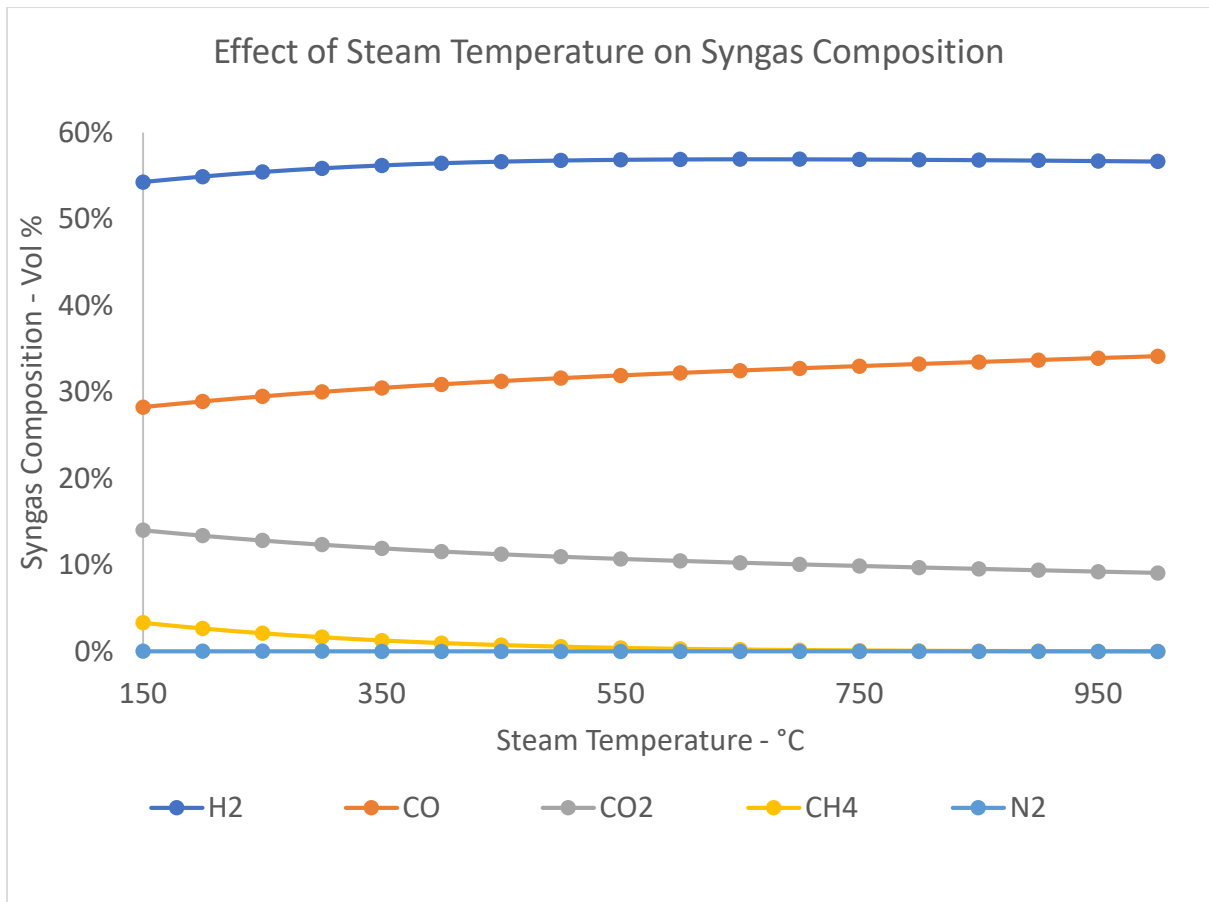


Figure 4-2: Effect of steam temperature on syngas composition for Sugarcane Bagasse feedstock

As shown on figure 4-2 when the steam temperature is increased from 150 – 1000 °C for Sugarcane Bagasse feedstock, both H₂ and CO increases. H₂ increase from 54,28 % to 56,67 % while CO increase from 28,27 % to 34,15 %. On the contrary, both CO₂ and CH₄ drops. CO₂ drops from 14,05 % to 9,10 % and CH₄ drops from 3,35 % to 0,03 %. N₂ also drops from 0,05 % to 0,04 %.

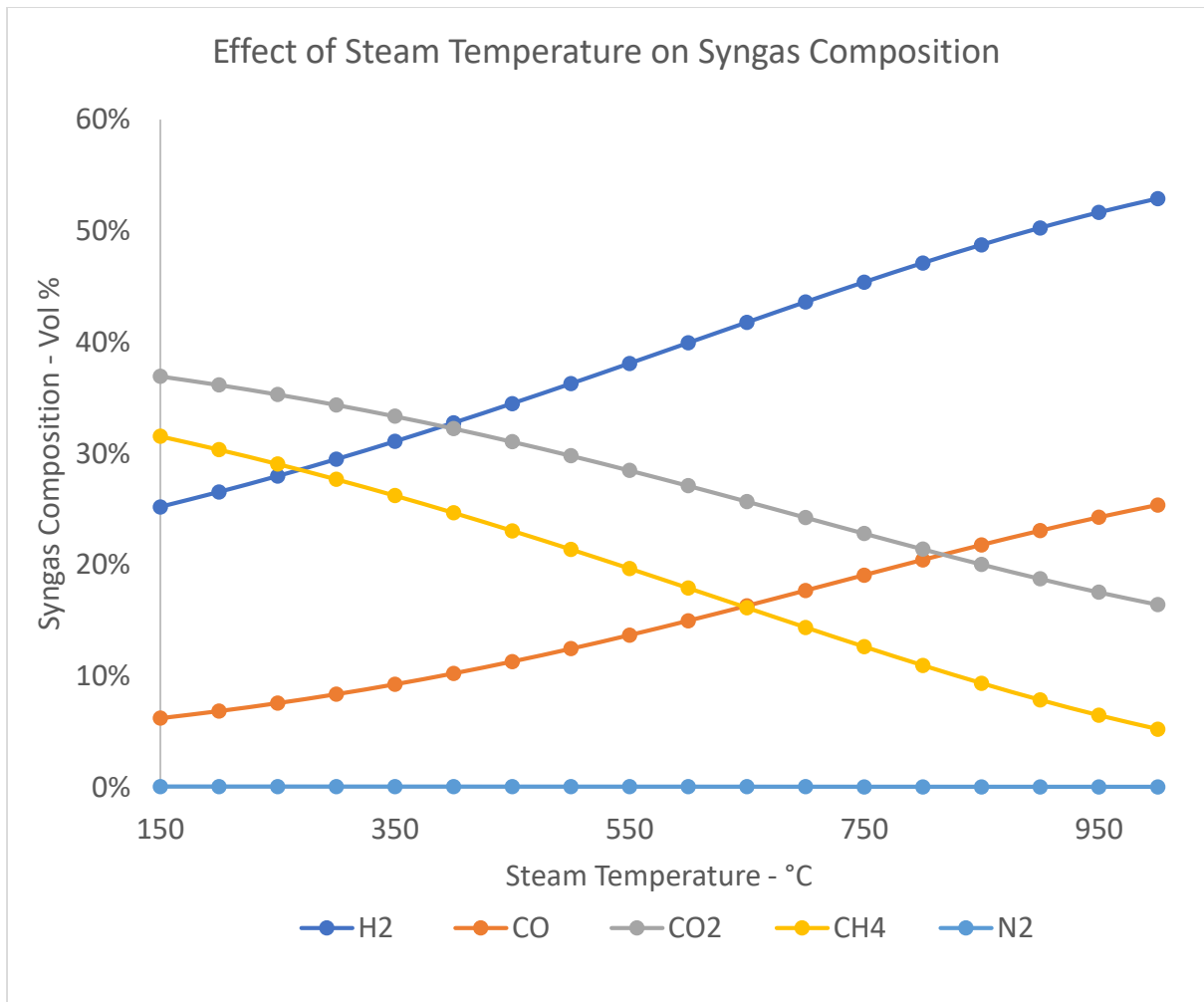


Figure 4-3: Effect of steam temperature on syngas composition for Rice Husk feedstock

As shown on figure 4-3 when the steam temperature is increased from 150 – 1000 °C for Rice Husk feedstock, both H₂ and CO increases. H₂ increase from 25,21 % to 52,90 % while CO increase from 6,23 % to 25,37 %. Contrary, both CO₂ and CH₄ drops. CO₂ drops from 36,93 % to 16,43 % and CH₄ drops from 31,54 % to 5,25 %. N₂ also drops from 0,09 % to 0,05 %.

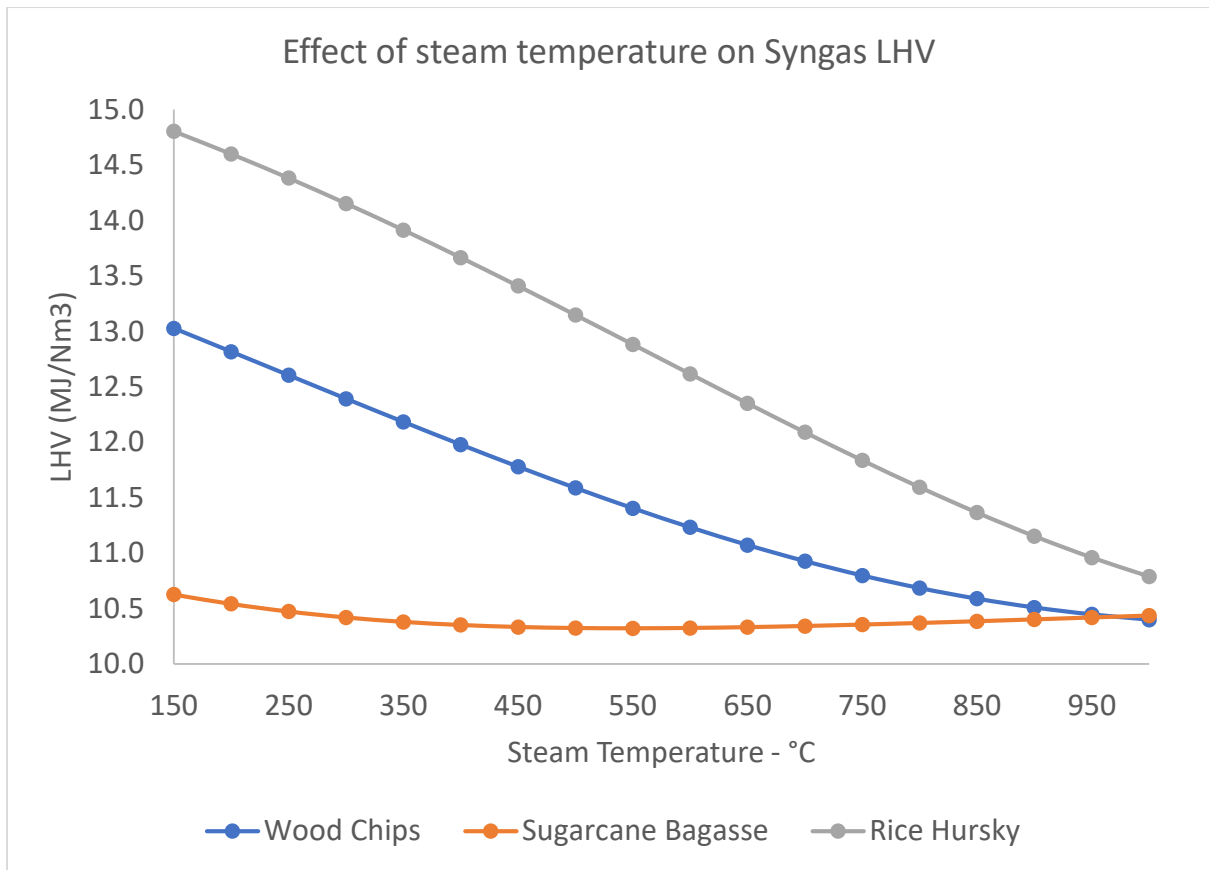


Figure 4-4: Effect of steam temperature on LHV of syngas for Wood Chips, Sugarcane Bagasse and Rice Husk feedstock

As shown on figure 4-4 as the steam temperature increases from 150 – 1000 °C, the LHV of syngas decreases from 13,03 to 10,40 MJ/Nm³ for Wood Chips, from 10,63 to 10,44 MJ/Nm³ for Sugarcane Bagasse and from 14,80 to 10,79 MJ/Nm³ for Rice Husk.

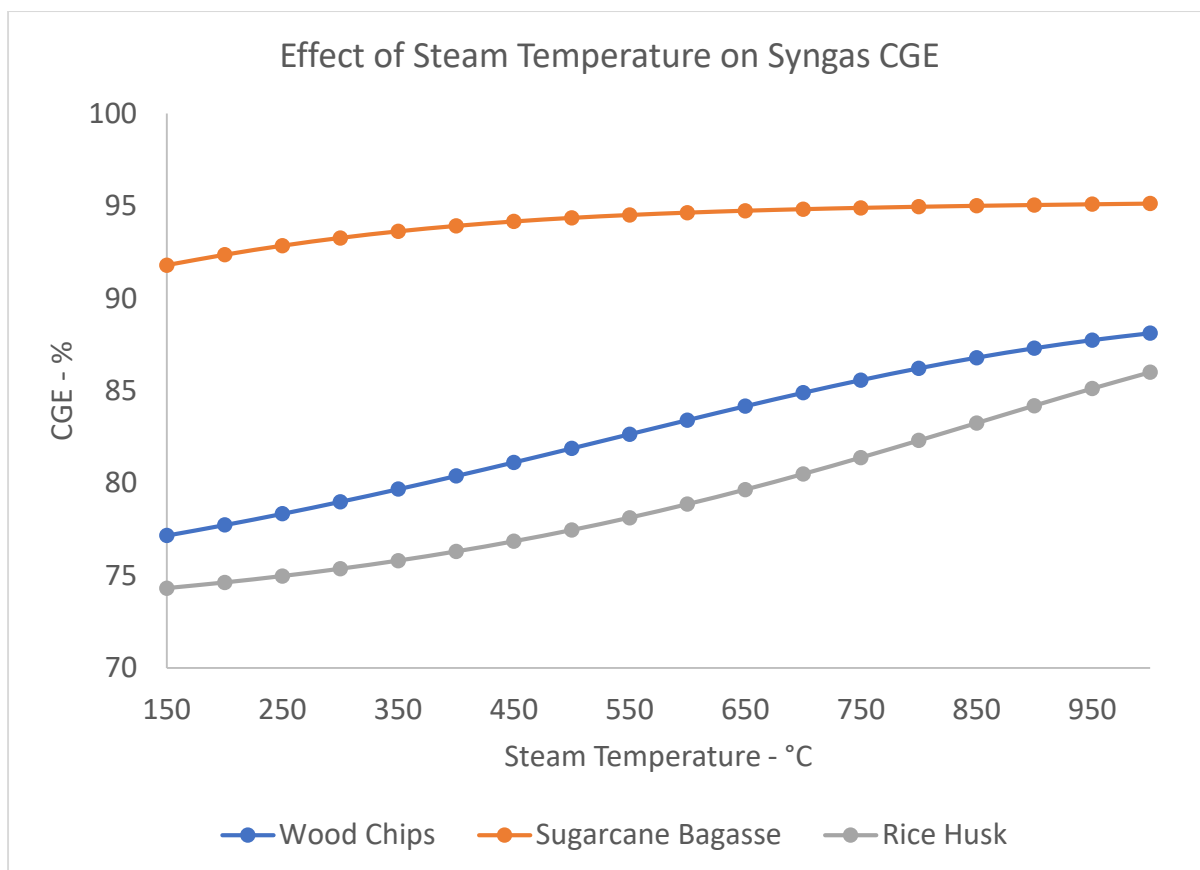


Figure 4-5: Effect of steam temperature on CGE for Wood Chips, Sugarcane Bagasse and Rice Husky feedstocks

The effect of steam temperature on CGE is illustrated on figure 4-5. As steam temperature is varied from 150 – 1000 °C, CGE increase from 77,17 % to 88,10 % for Wood Chip feed, from 91,13 % to 95,13 % for Sugarcane Bagasse feed and from 74,32 % to 86,00 % Rice Husk feed.

4.3 Sensitivity Analysis: Effect of Gasifier Temperature

In this case, the gasifier temperature was varied from 700 – 1100 °C while other input variables were held constant. The effect of gasifier temperature on syngas composition, syngas LHV and CGE for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks was studied.

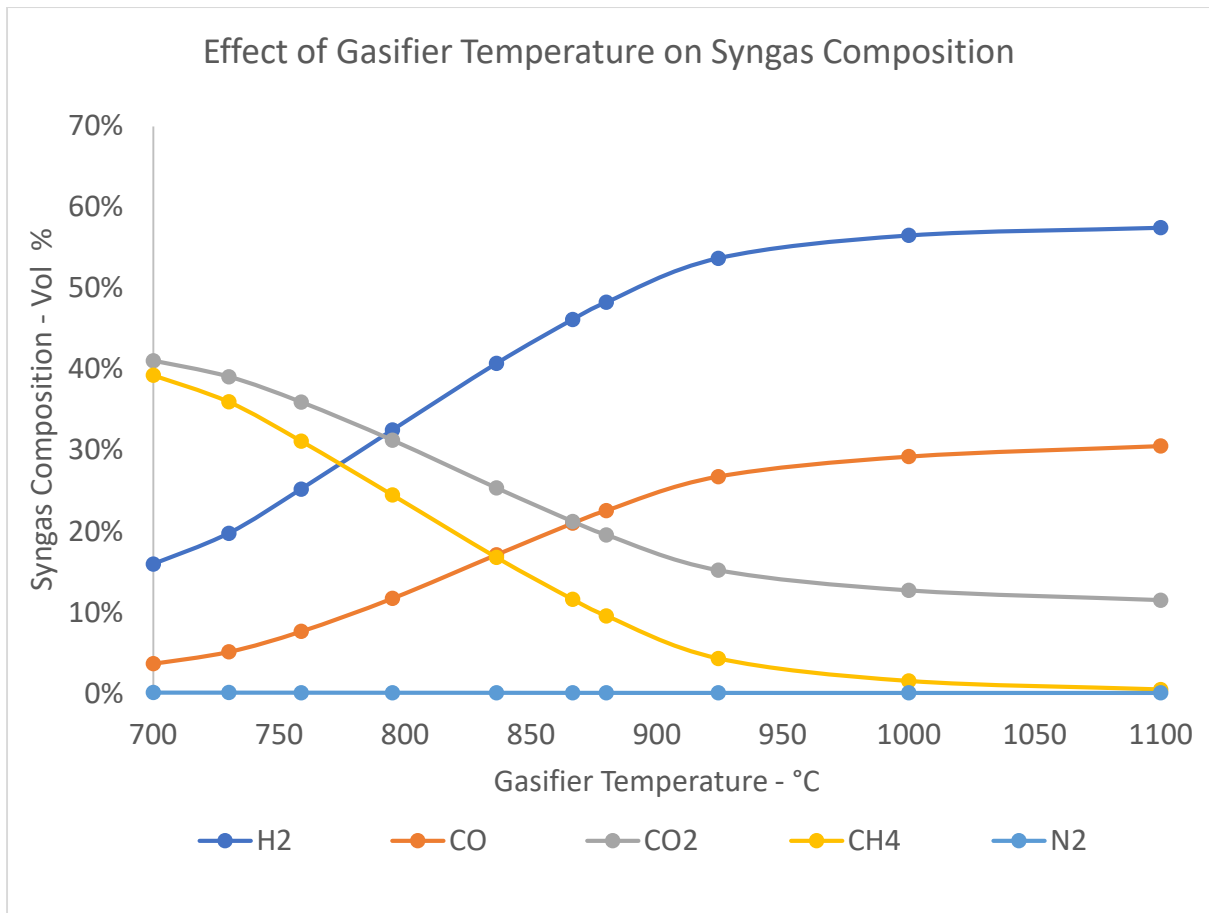


Figure 4-6: Effect of gasifier temperature on syngas composition for Wood Chips feedstock

As shown on figure 4-6, as the gasifier temperature increases from 700 – 1100 °C for Wood Chips feedstock, both H₂ and CO increases. H₂ increase from 15,95 % to 56,53 % while CO increase from 3,65 % to 29,22 %. On the contrary, both CO₂ and CH₄ decreases. CO₂ decrease from 41,05 % to 12,69 % while CH₄ decrease from 39,26 % to 1,54 %. N₂ content is low at 0,08 % – 0,05 %.

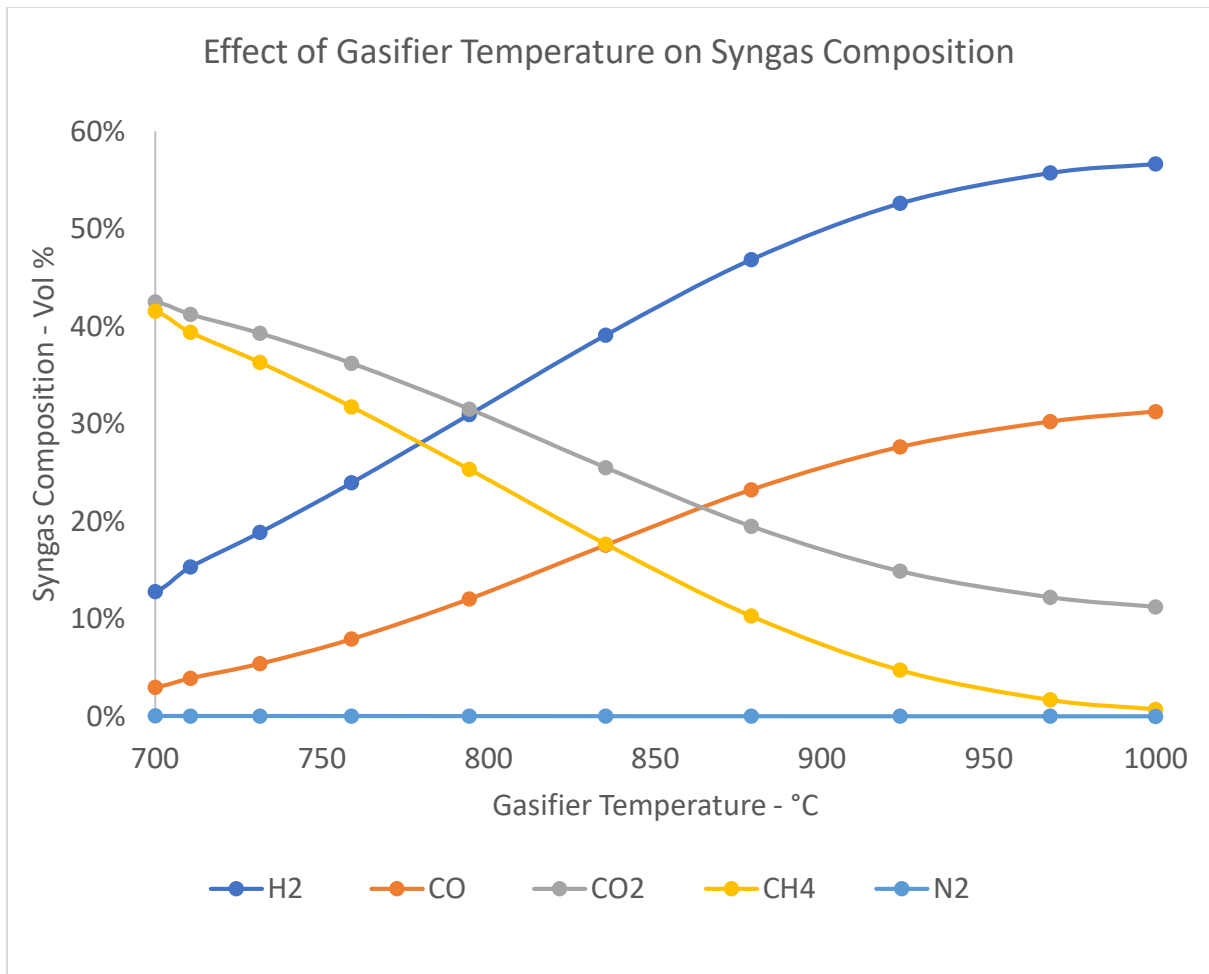


Figure 4-7: Effect of gasifier temperature on syngas composition for Sugarcane Bagasse feedstock

Figure 4-7 shows that as the gasifier temperature increase from 700 – 1000 °C for Sugarcane Bagasse feedstock, H₂ increase from 12,82 % to 56,66 % while CO increase from 3,02 % to 31,28 %. CO₂ decrease from 42,52 % to 11,26 % while CH₄ decrease from 41,56 % to 0,76 %. N₂ decrease from 0,08 % to 0,04 %.

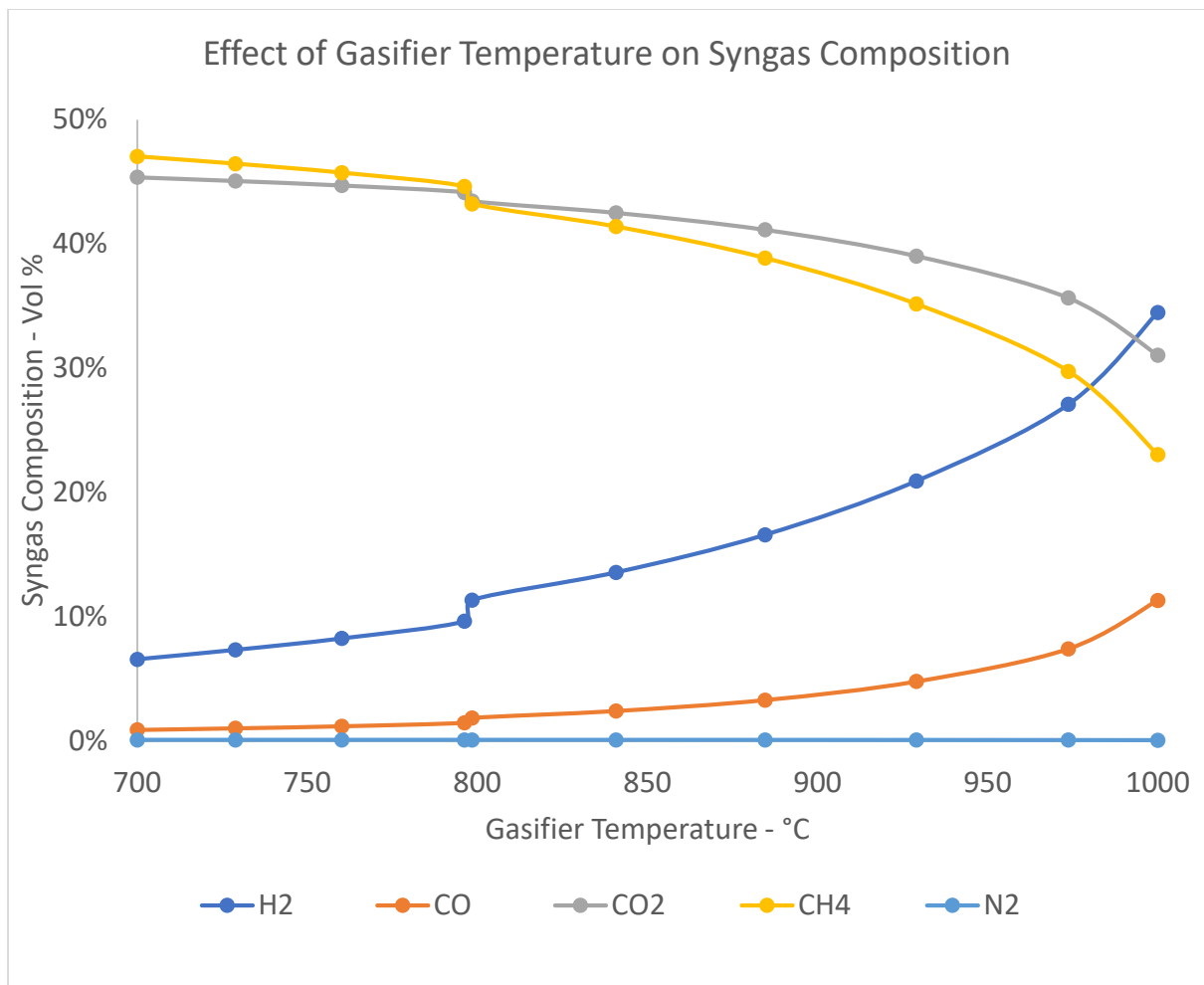


Figure 4-8: Effect of gasifier temperature on syngas composition for Rice Husk feedstock

Figure 4-8 shows that as the gasifier temperature increase from 700 – 1 000 °C for Rice Husk feedstock, both H₂ and CO increases. H₂ increase from 16,60 % to 58,13 % while CO increase from 3,30 % to 29,14 %. On the contrary, both CO₂ and CH₄ decreases. CO₂ decrease from 41,14 % to 12,35 % while CH₄ decrease from 38,87 % to 0,33 %. N₂ drops from 0,09 to 0,05 %.

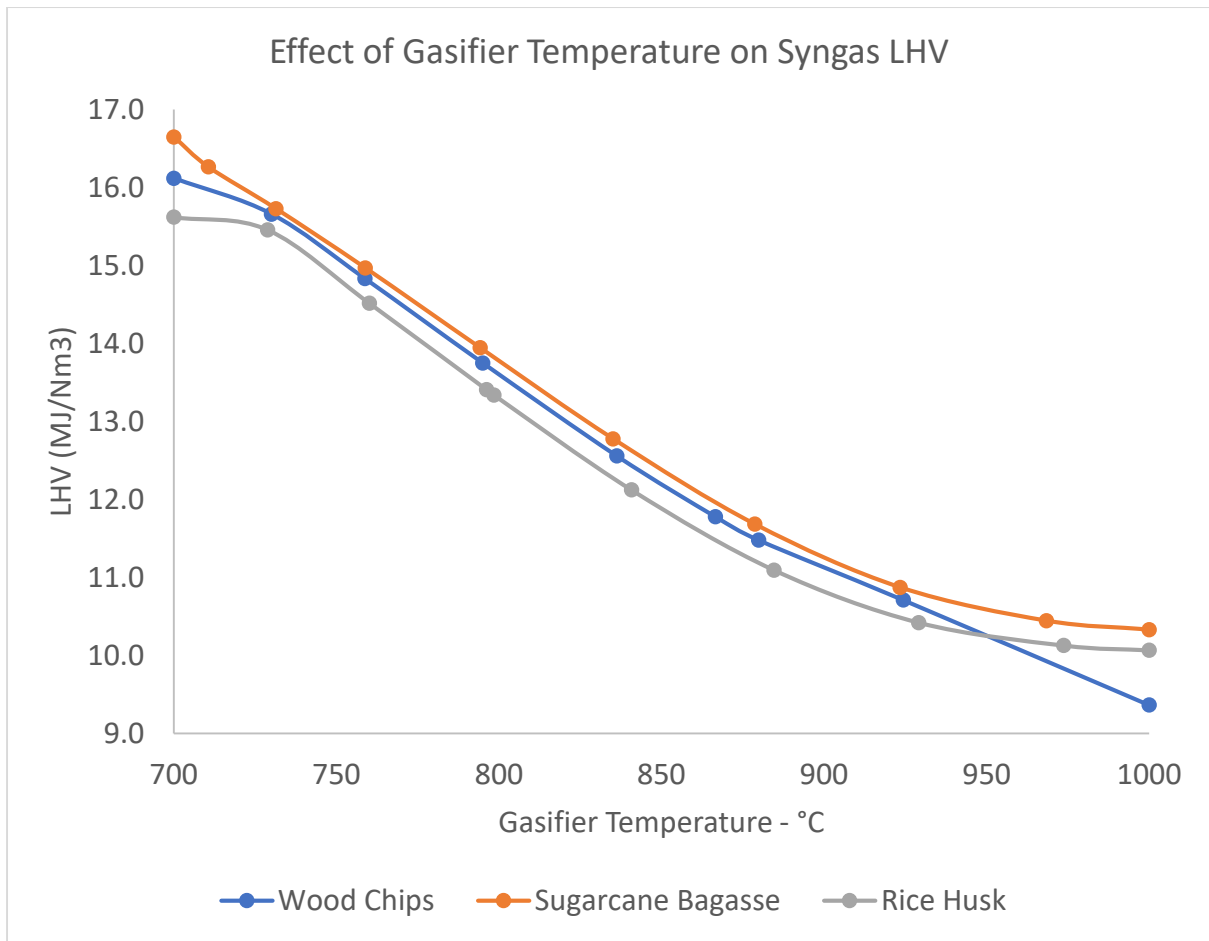


Figure 4-9: Effect of gasifier temperature on LHV of syngas composition for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of gasifier temperature on LHV of syngas for Wood Chips, Sugarcane Bagasse and Rice Husk feedstock is shown on figure 4-9. As the gasifier temperature increase from 700 – 1 000 °C, syngas LHV drops from 16,12 to 9,37 MJ/Nm³ for Wood Chips feedstock, from 16,65 to 10,33 MJ/Nm³ for Sugarcane Bagasse feedstock, from 15,62 to 10,07 MJ/Nm³ for Rice Husk feedstock.

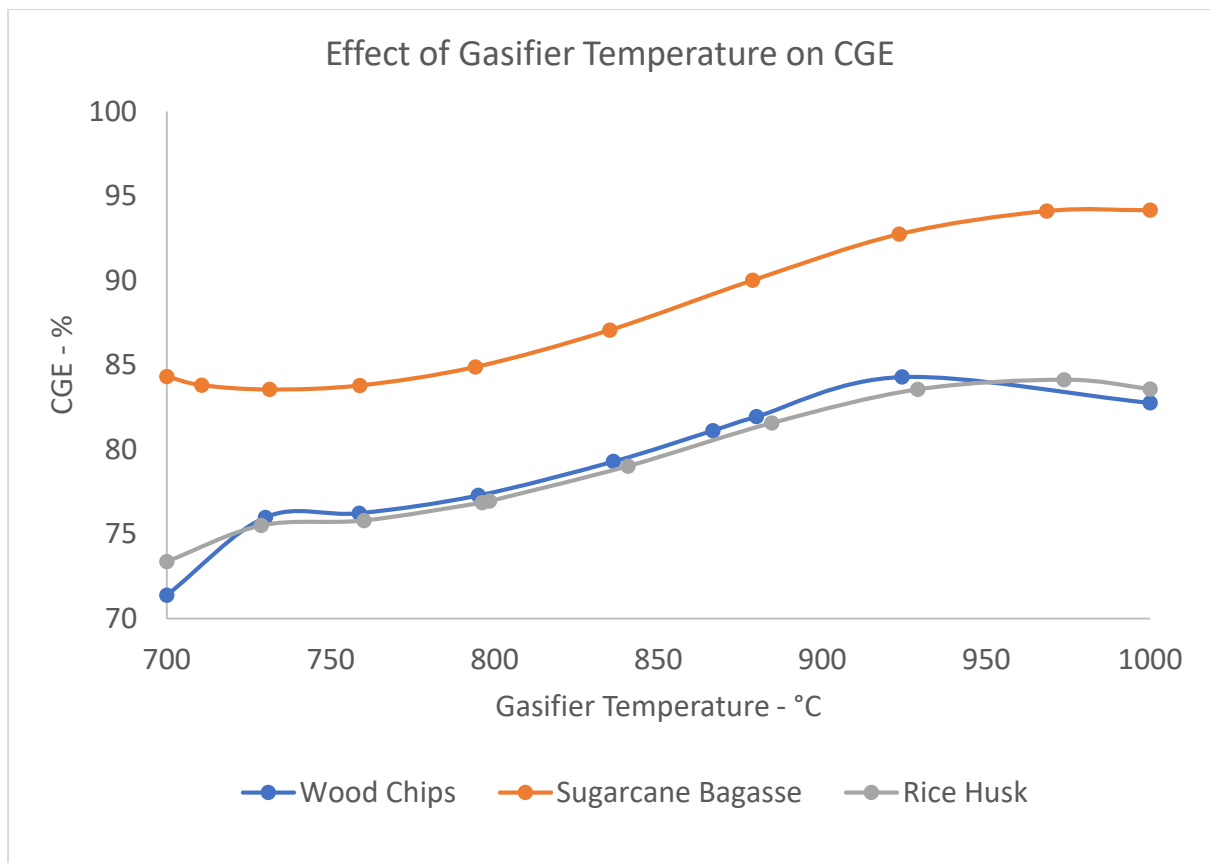


Figure 4-10: Effect of gasifier temperature CGE for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of gasifier temperature on CGE is shown on figure 4-10. As the gasifier temperature increases from 700 – 1 000 °C CGE increase from 71,38 % to 82,76 % for Wood Chips feedstock, from 84,32 % to 94,16 % for Sugarcane Bagasse feedstock and from 73,37 % to 83,58 % for Rice Husk feedstock.

4.4 Sensitivity Analysis: Effect of Steam to Feed Ratio

In this case, steam to feed ratio was varied from 0,4 to 1,0 while other parameters were held constant. The syngas gas composition on dry basis, LHV of syngas and CGE was studied.

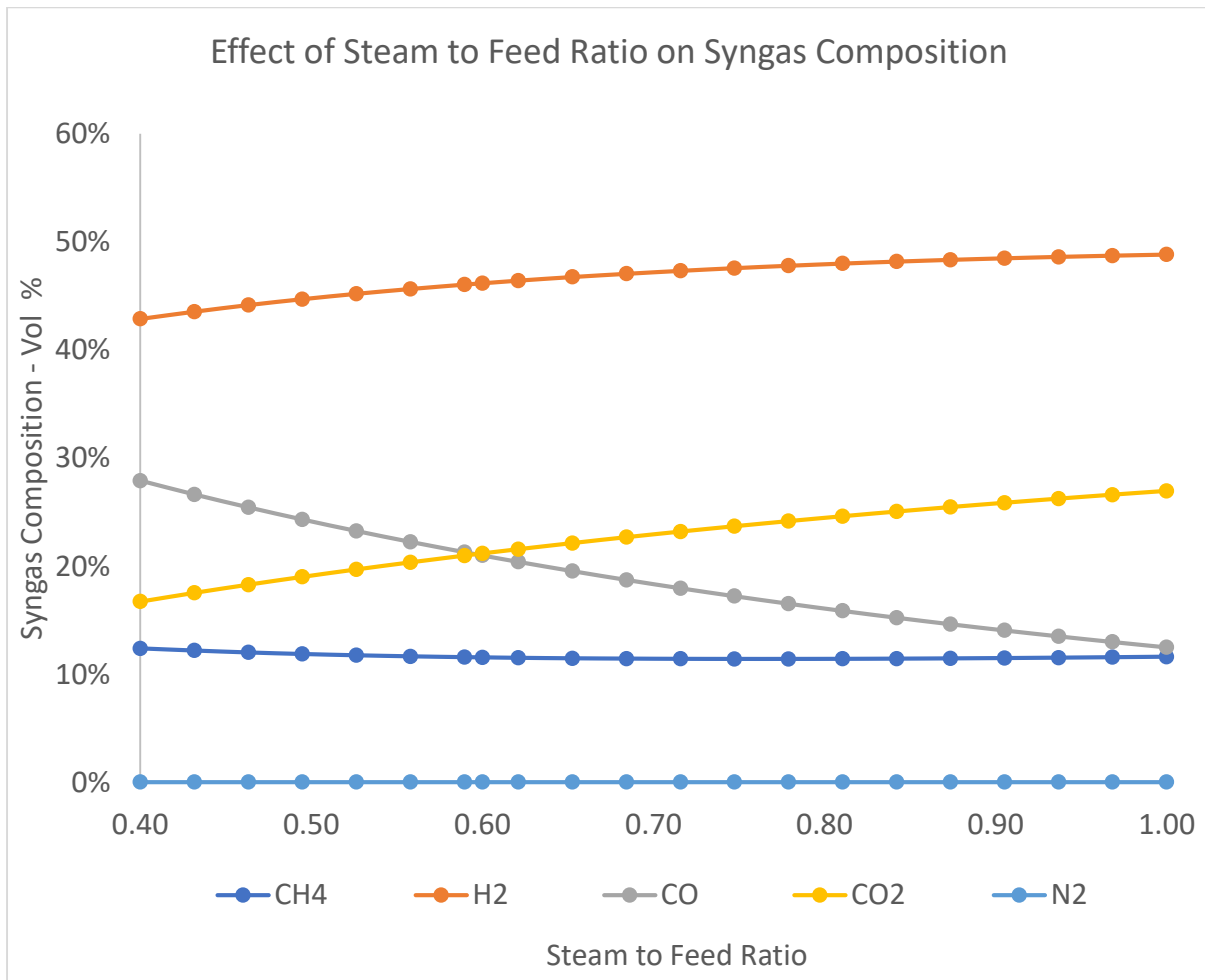


Figure 4-11: Effect of steam to feed ratio on syngas composition for Wood Chips feedstock

Figure 4-11 shows that as the steam to feed ratio for Wood Chips feedstock is increased from 0,4 to 1,0, H₂ increase from 42,88 % to 48,82 %. CO drops from 27,91 % to 12,52 %. CO₂ increases while CH₄ decreases. CO₂ increase from 16,74 % to 26,97 %, CH₄ decrease from 12,41 % to 11,64 %. N₂ content is low at 0,05 – 0,05 %.

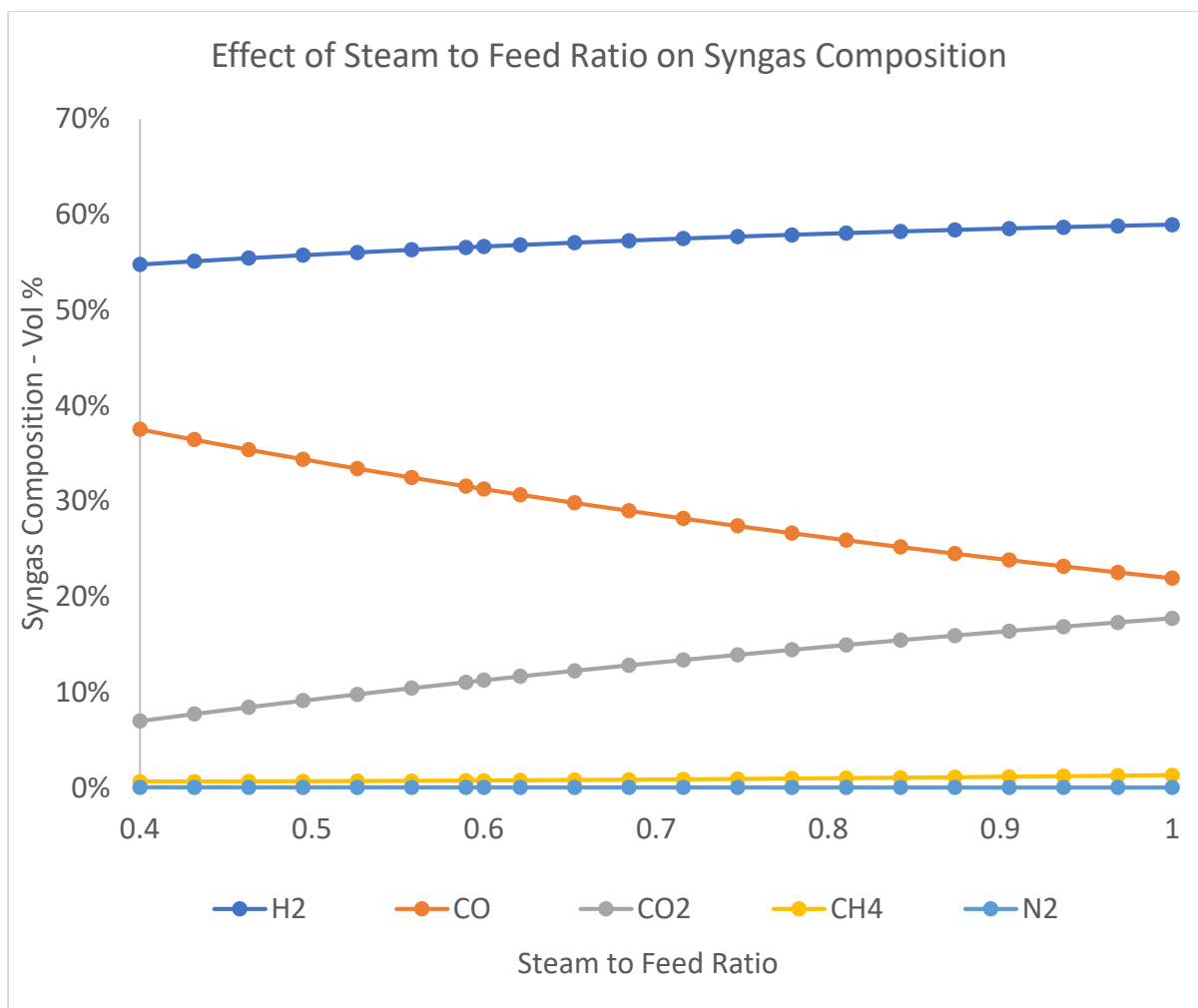


Figure 4-12: Effect of steam to feed ratio on syngas composition for Sugarcane Bagasse feedstock

Figure 4-12 shows that as the steam to feed ratio for Sugarcane Bagasse feedstock is increased from 0,4 to 1,0 H₂ increase from 54,78 % to 58,94 %. CO drops from 37,52 % to 21,94 %. CO₂ increase from 7,00 % to 17,75 %. Both CH₄ and N₂ are low at 0,66 – 1,32 % and 0,04 - 0,05 %.

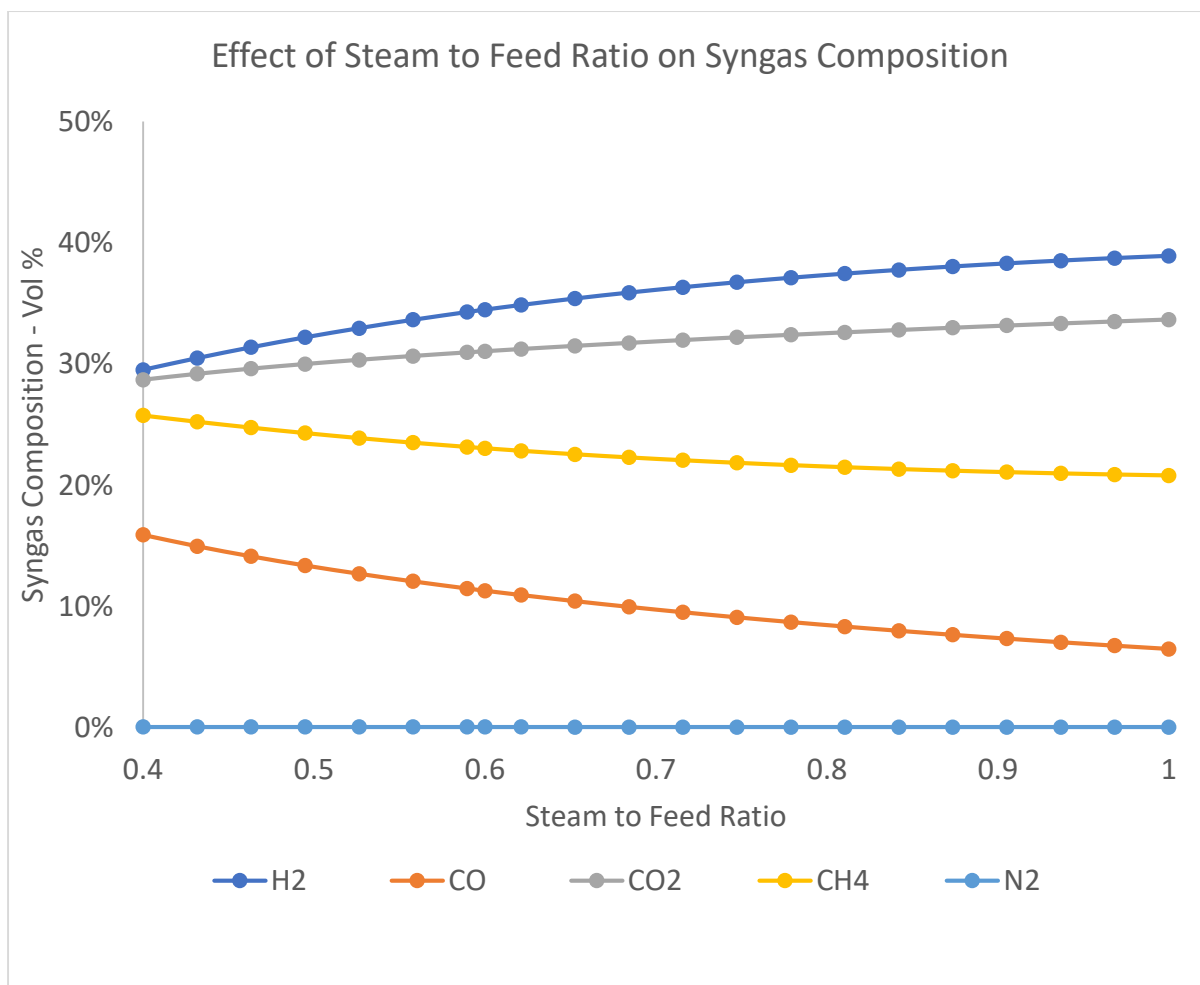


Figure 4-13: Effect of steam to feed ratio on syngas composition for Rice Husk feedstock

Figure 4-13 shows that as the steam to feed ratio for Rice Husk feedstock is increased from 0,4 to 1,0 H₂ increase from 29,53 % to 38,92 %. CO drops from 15,92 % to 6,51 %. CO₂ increase while CH₄ decreases. CO₂ increase from 28,71 % to 33,68 %, CH₄ decrease from 25,76 % to 20,82 %. N₂ content is low at 0,07 – 0,08 %.

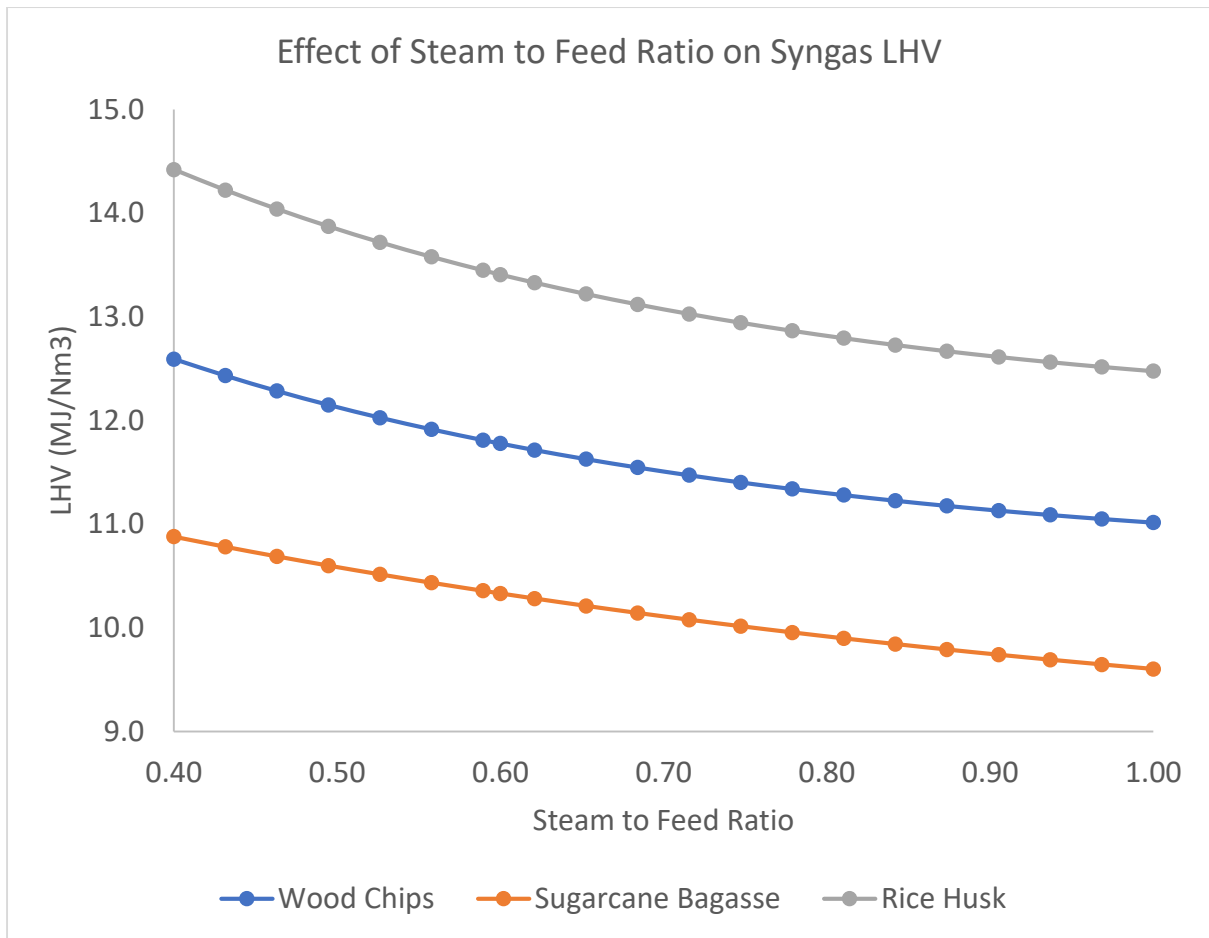


Figure 4-14: Effect of steam to feed ratio on LHV of syngas composition for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of steam to feed ratio on LHV of syngas is illustrated on figure 4-14. With the steam to feed ratio increasing from 0,4 to 1,0 the LHV for all 3 feedstocks decreases. For Wood Chips feedstock it decreases from 12,59 to 11,02 MJ/Nm³. For Sugarcane Bagasse feedstock the LHV decrease from 10,88 to 9,60 MJ/Nm³. Lastly, the LHV of syngas for Rice Husk feedstock decreases from 14,42 to 12,48 MJ/Nm³.

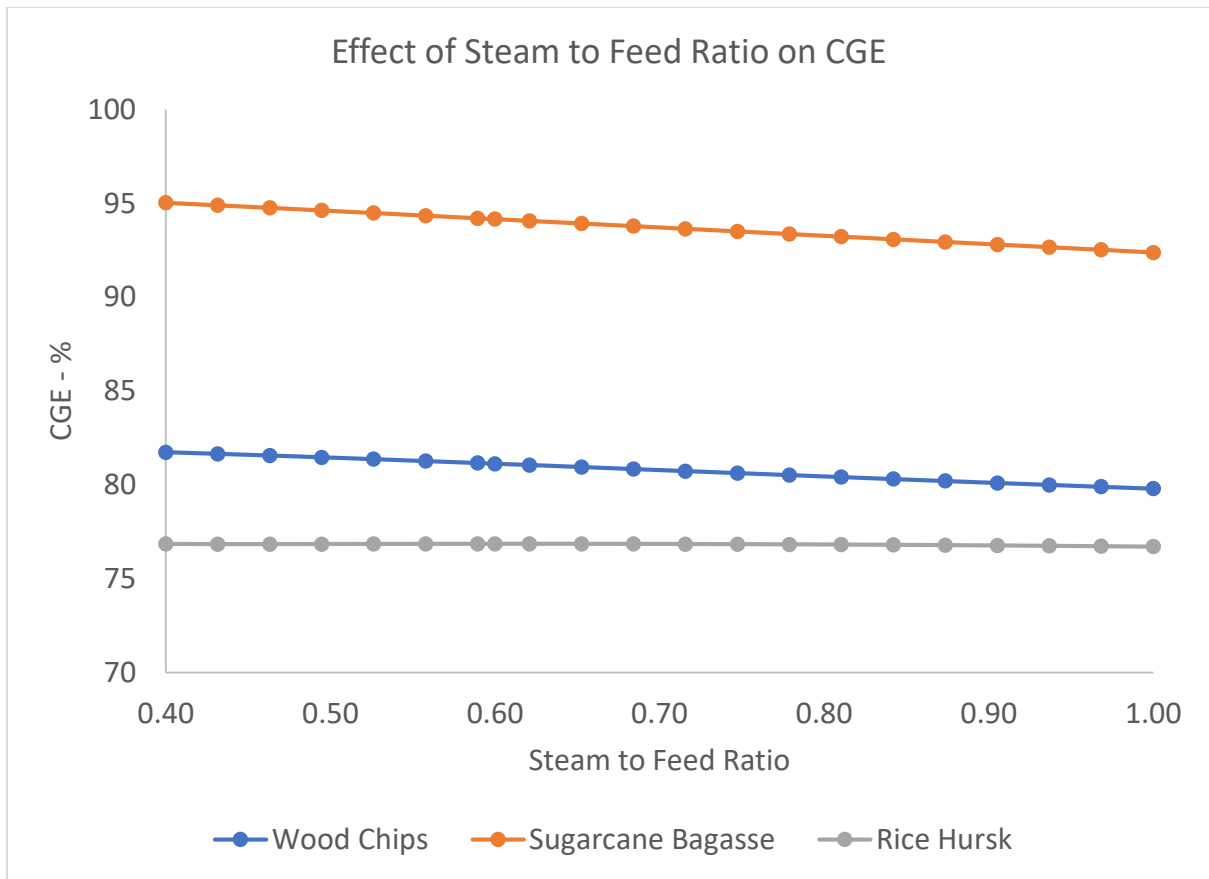


Figure 4-15: Effect of steam to feed ratio on Cold Gasification Efficiency for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of steam to feed ratio on CGE is shown on figure 4-15. As steam to feed ratio is varied from 0,4 – 1,0 CGE decrease from 81,73 % to 79,80 % for Wood Chips feedstock, from 95,03 % to 92,38 % for Sugarcane Bagasse feed, and from 76,85 % to 76,71 % for Rice Husk feedstock.

4.5 Sensitivity Analysis: Effect of Combustion Air Temperature

In this instance, the combustion air temperature was varied from 25 to 1 000 °C while other parameters were held constant. The syngas gas composition on dry basis, LHV of syngas and CGE was studied.

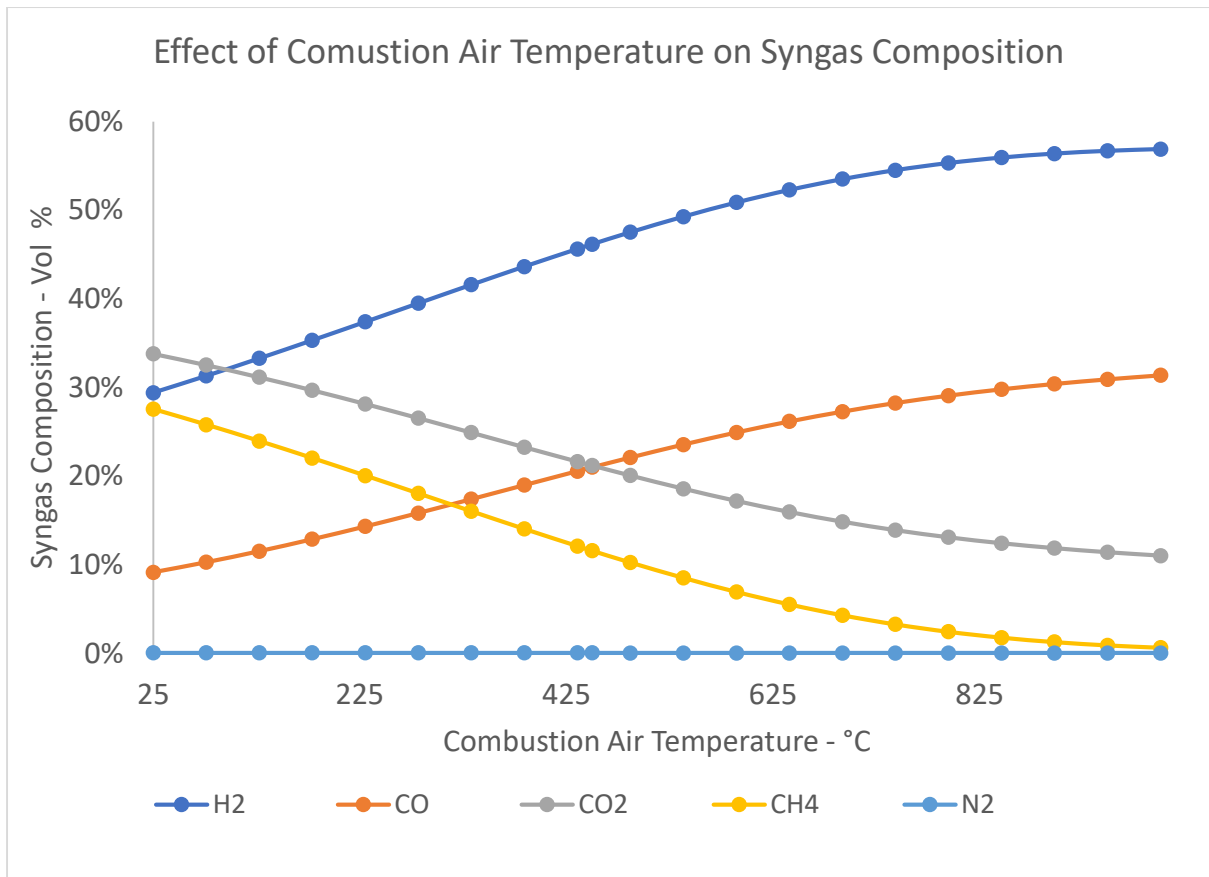


Figure 4-16: effect of combustion air temperature on syngas composition for Wood Chips feedstock

As seen on figure 4-16, as the combustion air temperature increase from 25 – 1000 °C, both H₂ and CO increases. H₂ increases from 29,42 % to 56,90 % while CO increase from 9,15 % to 31,38 %. On the contrary, both CO₂ and CH₄ decreases. CO₂ decrease from 33,80 % to 11,03 % while CH₄ decrease from 27,56 % to 0,65 %. N₂ content is very low at 0,04 % – 0,07 %

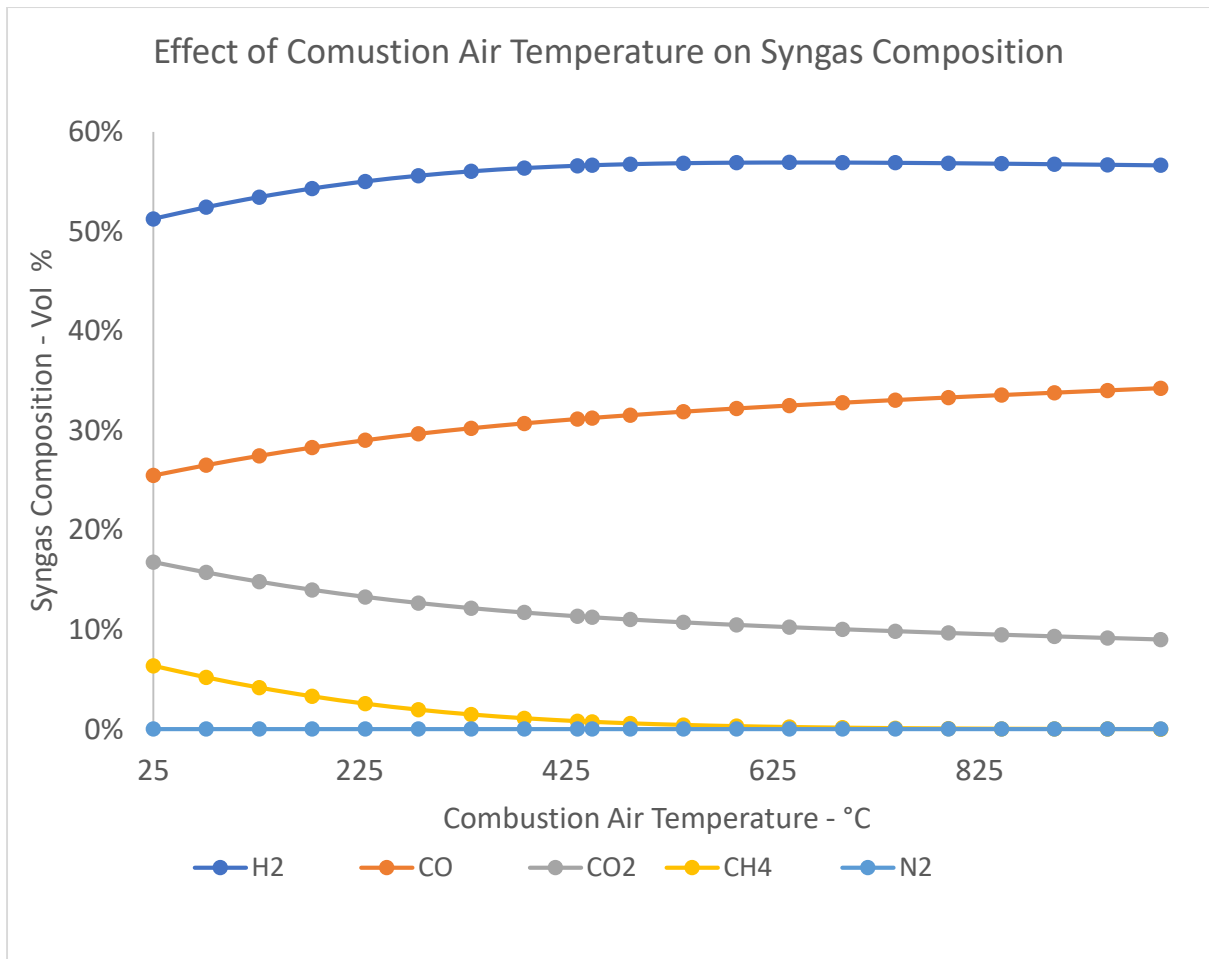


Figure 4-17: Effect of combustion air temperature on syngas composition for sugarcane bagasse feedstock

As seen on figure 4-17, as the combustion air temperature increase from 25 – 1000 °C, both H₂ and CO increases. H₂ from 51,26 % to 56,64 % while CO increase from 25,50 % to 34,25 %. On the contrary, both CO₂ and CH₄ decreases. CO₂ decrease from 16,81 % to 9,03% while CH₄ decrease from 6,39 % to 0,03 %. N₂ content is very low at 0,04 % – 0,05 %.

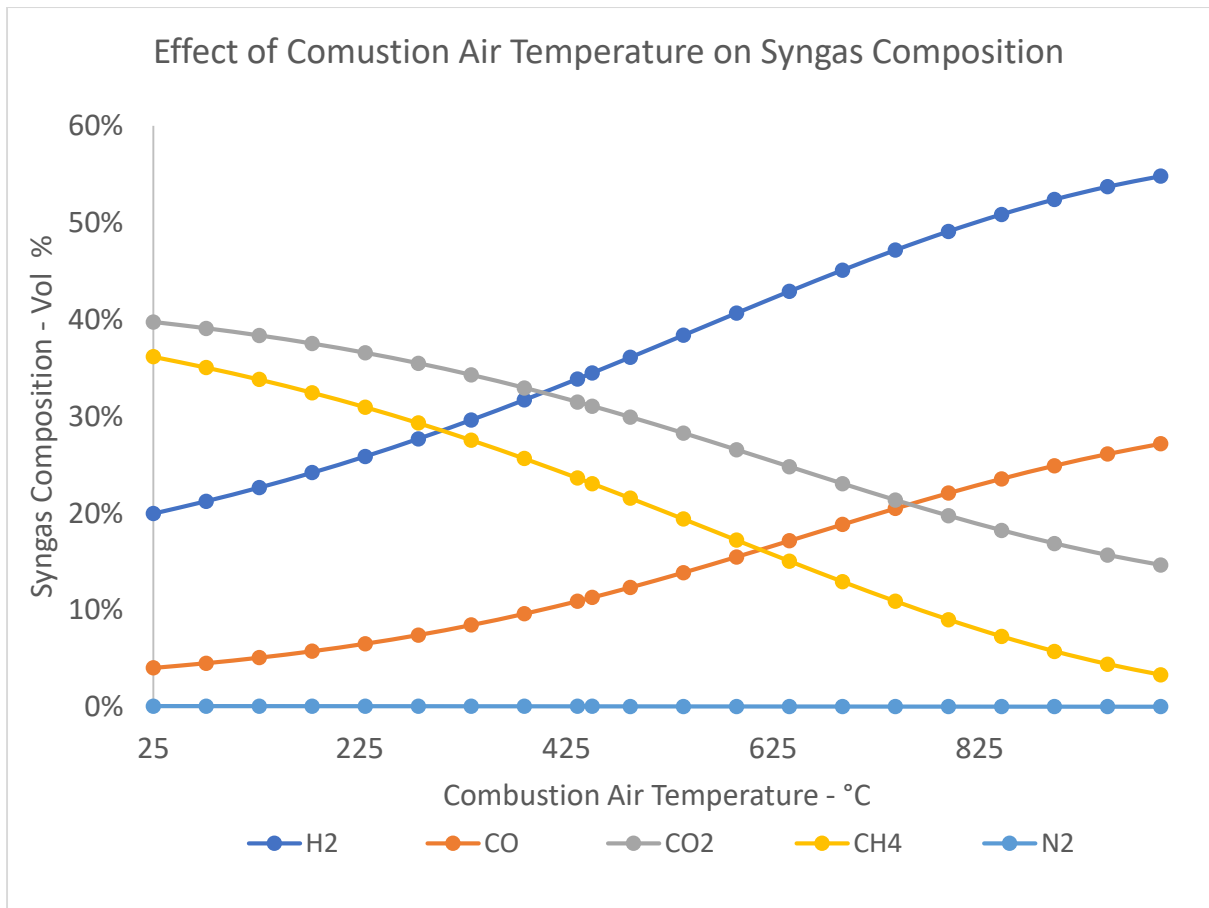


Figure 4-18: Effect of combustion air temperature on syngas composition for Rice Husk feedstock

As seen on figure 4-18, as the combustion air temperature increase from 25 – 1000 °C, both H₂ and CO increases. H₂ from 19,96 % to 54,78 % while CO increase from 4,04 % to 27,17 %. On the contrary, both CO₂ and CH₄ decreases. CO₂ decrease from 33,74 % to 14,66 % while CH₄ decrease from 36,16 % to 3,33 %. N₂ content is very low at 0,05 % – 0,09 %.

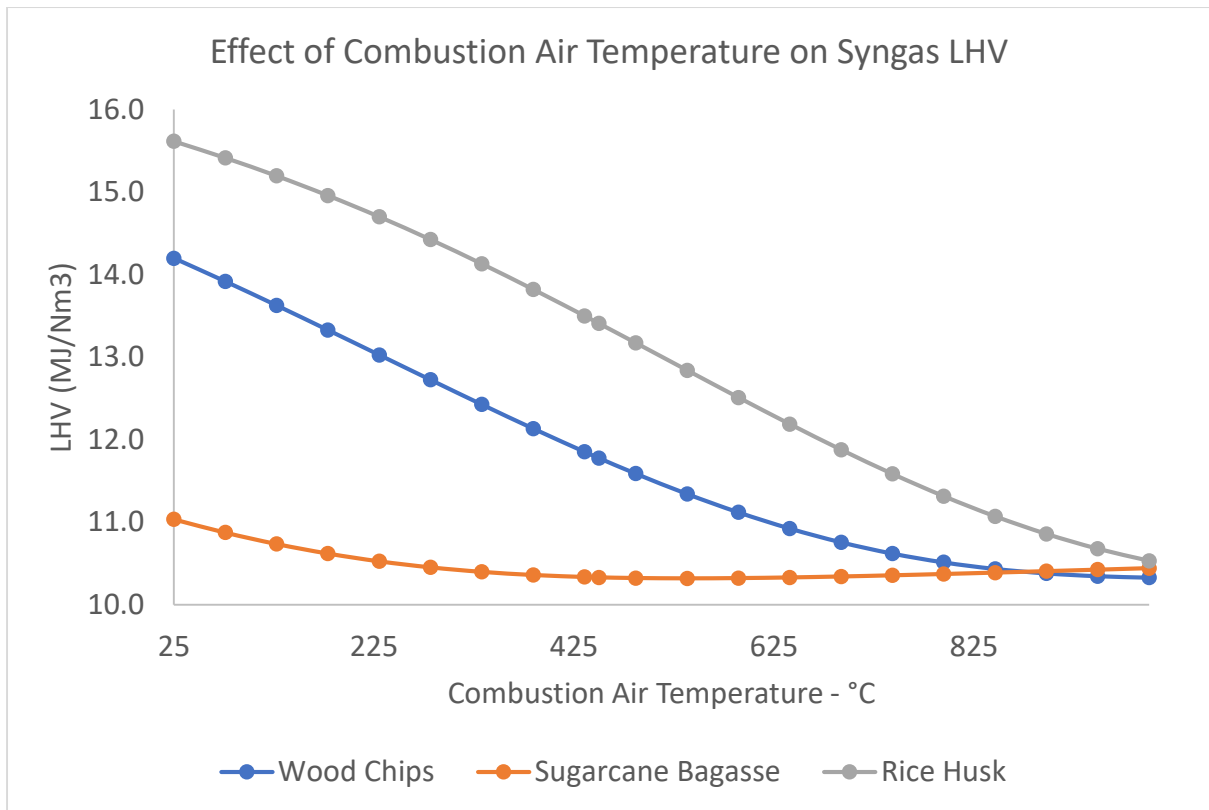


Figure 4-19: Effect of combustion air temperature on LHV of syngas composition for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of steam to feed ratio on LHV of syngas is illustrated on figure 4-19. With the combustion air temperature increasing from 25 to 1000 °C the LHV for all 3 feedstocks decreases. For Wood Chips feedstock it decreases from 14,20 to 10,33 MJ/Nm³. For Sugarcane Bagasse feedstock the LHV decrease from 11,04 to 10,44 MJ/Nm³. Lastly, the LHV of syngas for Rice Husk feedstock decreases from 15,61 to 10,53 MJ/Nm³.

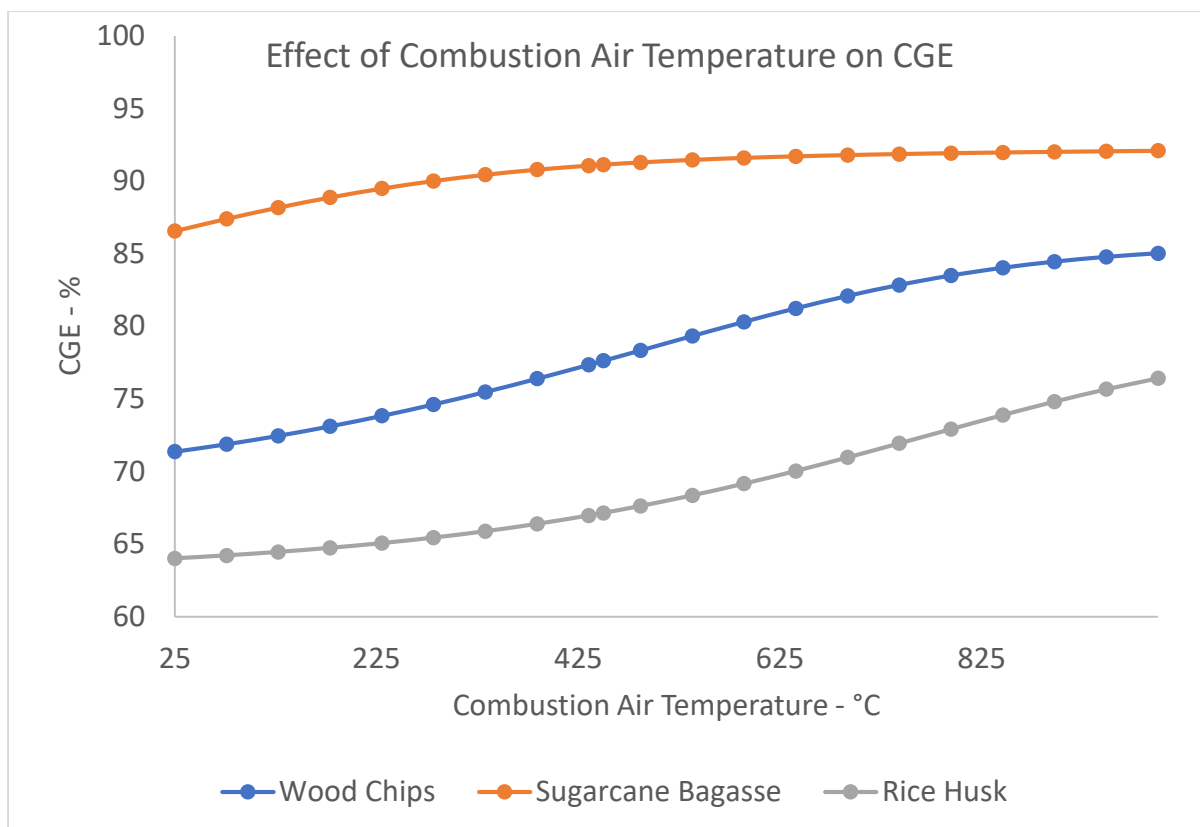


Figure 4-20: Effect of combustion air temperature on CGE for Wood Chips, Sugarcane Bagasse and Rice Husk feedstock s

The effect of combustion air temperature on CGE is shown on figure 4-20. As the combustion air temperature is varied from 25 – 1 000 °C the CGE increase from 71,37 % to 85,03 % for Wood Chips feedstock, from 86,57 % to 92,09 % for Sugarcane Bagasse feedstock, and from 64,01 % to 76,42 % for Rice Husk feedstock.

4.6 Sensitivity Analysis: Effect of Combustion Air to Feed Ratio

In this instance, air to feed ratio (on mass basis) was varied from 0,7 – 2,0 while other parameters were held constant. The effect of combustion air to feed ratio on dry syngas composition, syngas LHV as well as CGE was studied.

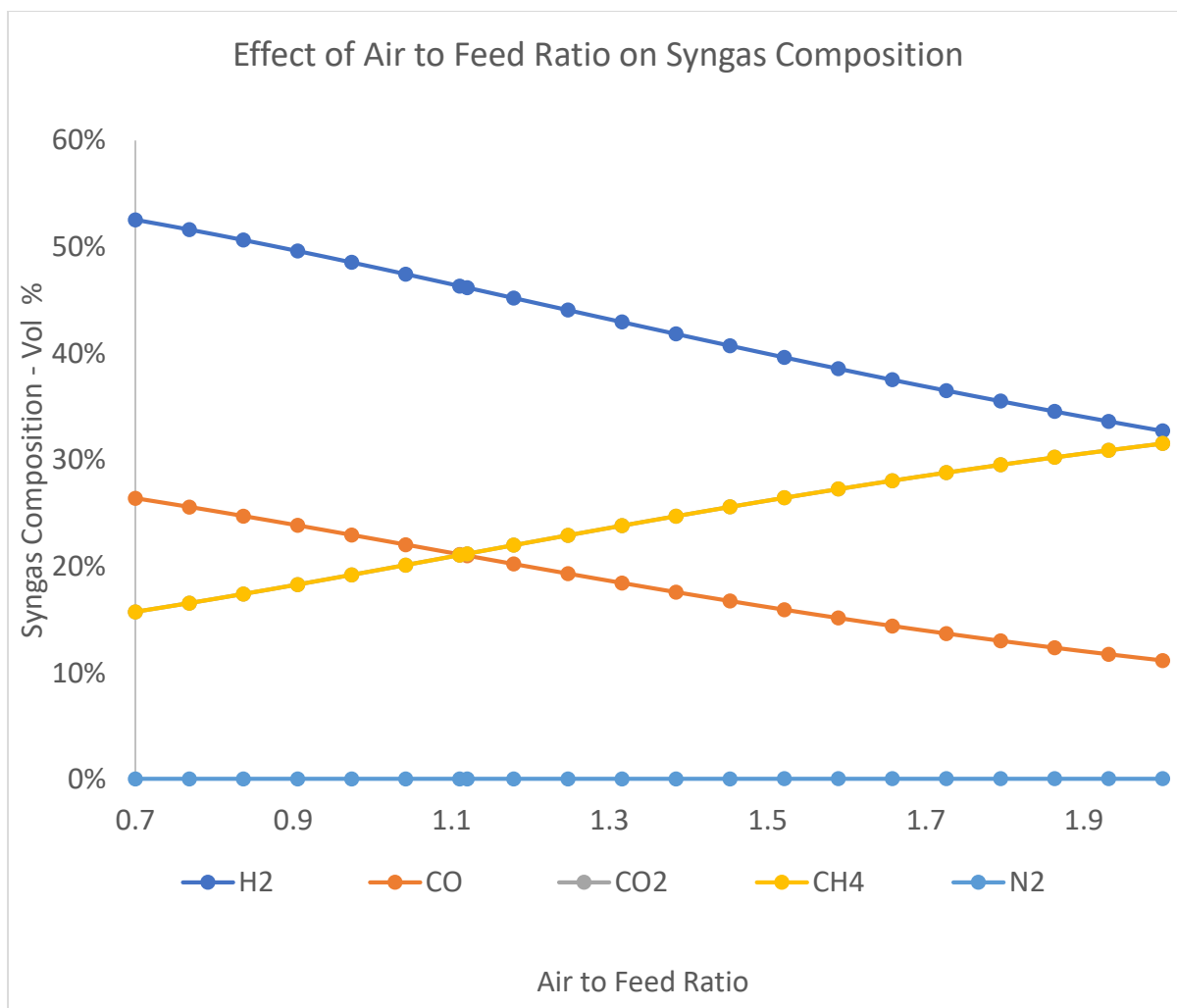


Figure 4-21: Effect of air to feed ratio on syngas composition for Wood Chips feedstock

Figure 4-21 shows that as the combustion air to feed increase from 0,7 - 2,0 both H₂ and CO decreases. H₂ decrease from 52,54 % to 32,73 % while CO decrease from 26,40 % to 11,17 %. On the contrary, both CO₂ and CH₄ increases. CO₂ increase from 15,73 % to 31,55 % while CH₄ increase from 5,28 % to 24,48 %. N₂ content is very low at 0,05 % – 0,07 %.

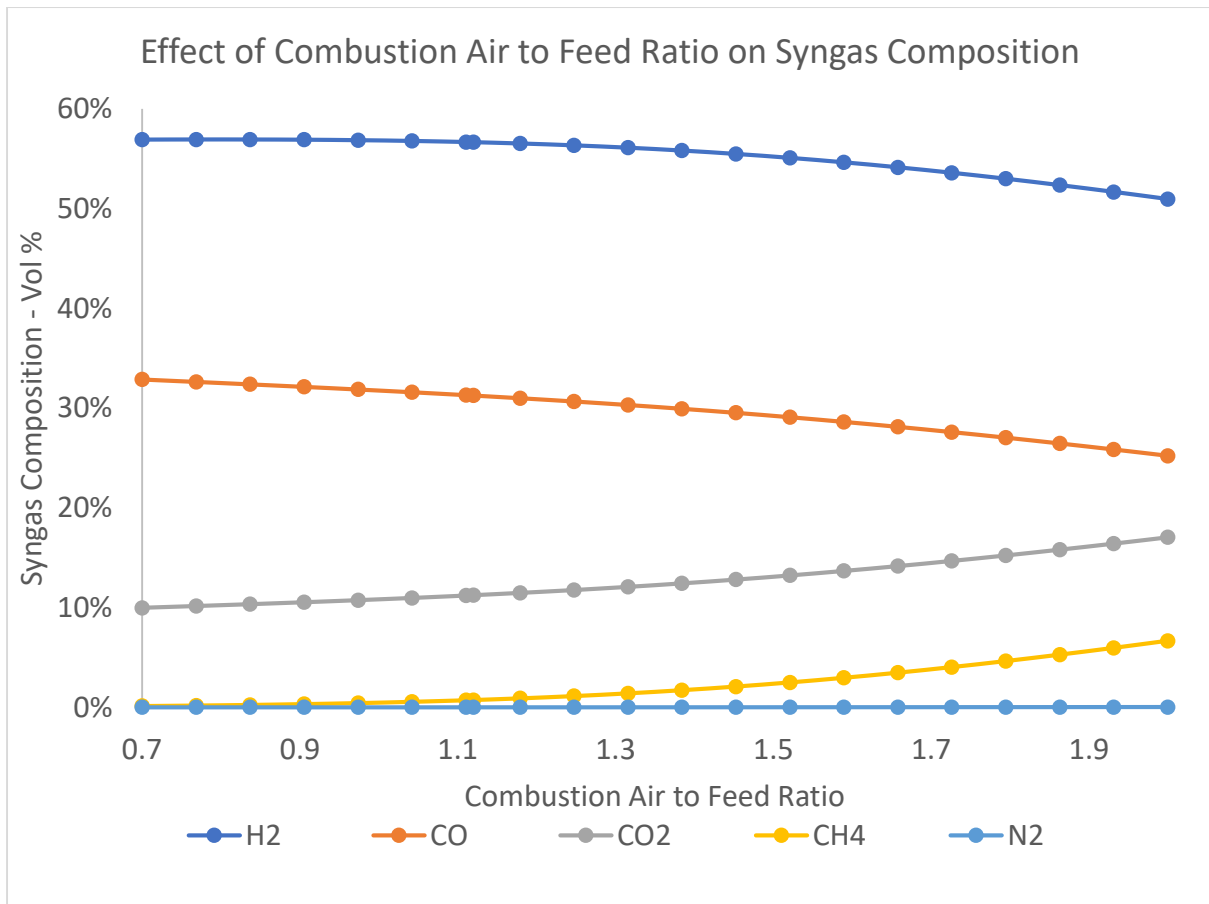


Figure 4-22: Effect of combustion air to feed on syngas composition for Sugarcane Bagasse feedstock

Figure 4-22 shows that as the combustion air to feed increase from 0,7 - 2,0 both H₂ and CO decreases. H₂ from 56,92 % to 50,95 % while CO decrease from 32,88 % to 25,23 %. On the contrary, both CO₂ and CH₄ increases. CO₂ increase from 10,00 % to 17,07 % while CH₄ increase from 0,16 % to 6,69 %. N₂ content is very low at 0,04 % – 0,05 %.

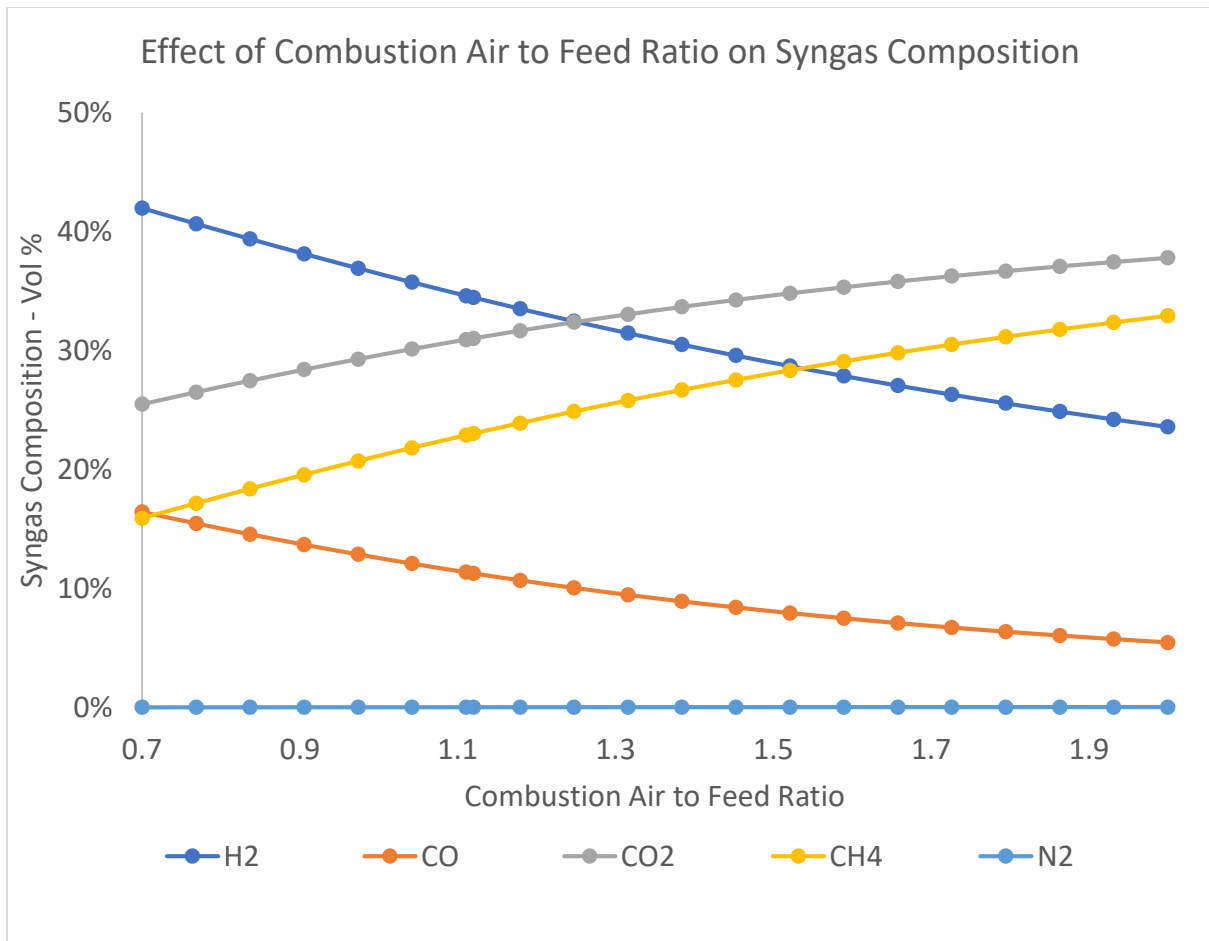


Figure 4-23: Effect of combustion air to feed ratio on syngas composition for Rice Husk feedstock

Figure 4-23 shows that as the combustion air to feed increase from 0,7 - 2, both H₂ and CO decreases. H₂ decrease from 41,99 % to 23,63 % while CO decrease from 16,48 % to 5,52 %. On the contrary, both CO₂ and CH₄ increases. CO₂ increase from 25,53 % to 37,82 % while CH₄ increase from 15,95 % to 32,95 %. N₂ content is very low at 0,07 % – 0,09 %.

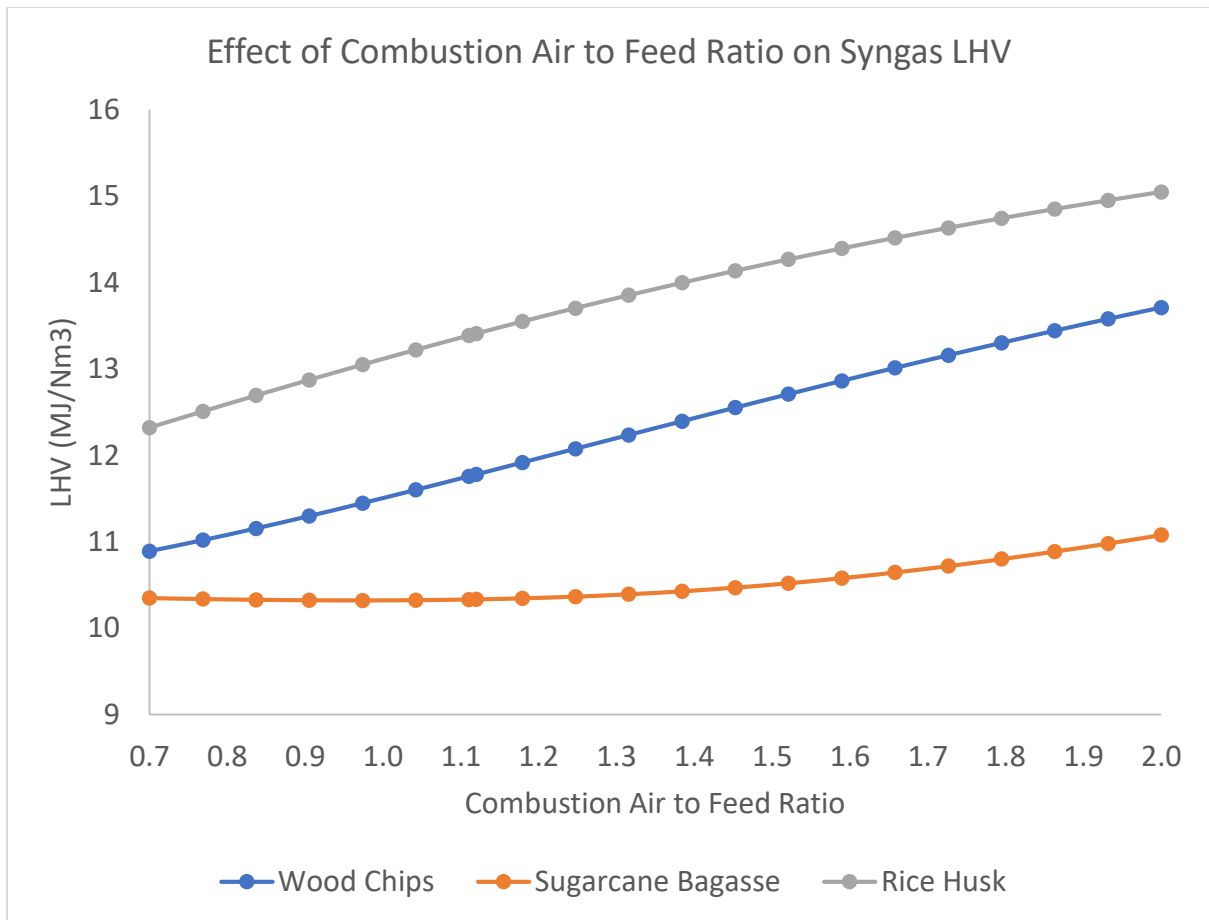


Figure 4-24: Effect of combustion air to feed ratio on LHV of syngas composition for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of combustion air to feed ratio on LHV of syngas is illustrated on figure 4-24. With the combustion air to feed ratio increasing from 0,7 to 2,0 the LHV for Wood Chips and Rice Husk gasification increases whereas LVH of Sugarcane Bagasse remain nearly constant. For Wood Chips feedstock LHV increases from 10,89 to 13,71 MJ/Nm³. Secondly, the LHV of syngas for Rice Husk feedstock decreases from 12,32 to 15,05 MJ/Nm³. Lastly, for the case of Sugarcane Bagasse feedstock the LHV increase slightly from 10,35 to 11,08 MJ/Nm³.

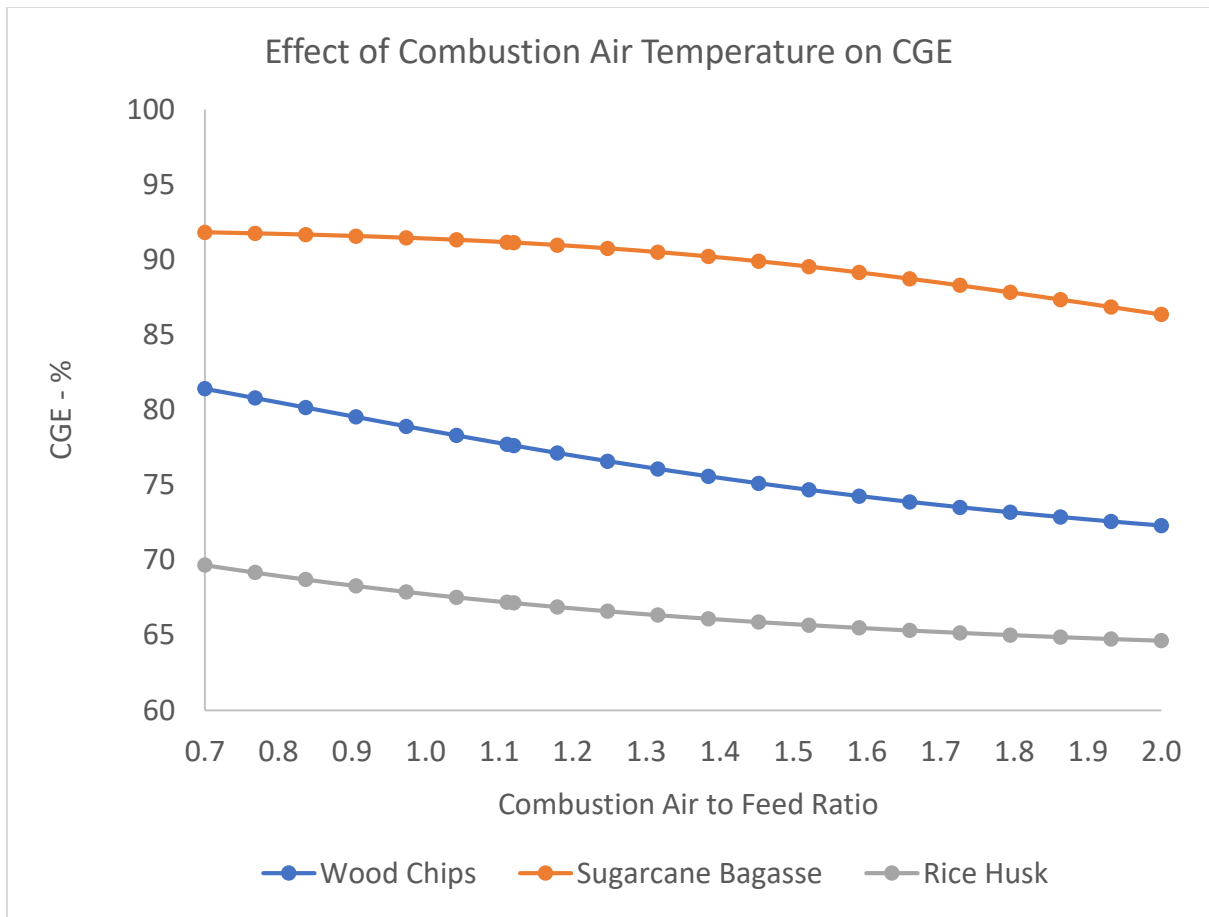


Figure 4-25: Effect of combustion air to feed ratio on Cold Gasification Efficiency for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The effect of combustion air to feed ratio on CGE is shown on figure 4-25. As combustion air to feed ratio is varied from 0,7 – 2,0, the CGE decrease from 81,41 % to 72,30 % for Wood Chips feedstock, from 91,82 % to 86,36 % for Sugarcane Bagasse feedstock, and from 69,67 % to 64,63 % for Rice Husk feedstock.

Chapter 5 Discussion

The results obtained from the sensitivity analysis are analysed and discussed in this section. The effect of steam temperature, gasifier temperature, steam to feed ratio, combustion air temperature and combustion air to feed ratio on gasification results for Wood Chips, Sugarcane Bagasse and Rice Husk are analysed and discussed in this section to determine the optimum gasification condition. The independent variables that were observed during the sensitivity analyses are syngas composition, syngas Lower Heating Value (LHV) and Cold Gasification Efficiency (CGE).

5.1 Steam Temperature

5.1.1 Effect of Steam Temperature on Syngas Composition

Figure 4-1, shows that as steam temperature during steam reforming of Wood Chips feedstock is increased from 150 – 1000 °C, both H₂ and CO increases by 18,83 % and 15,87 %, respectively. On the contrary, both CO₂ and CH₄ decrease by 16,08 % and 18,60 %, respectively.

The explanation for this observation is that as steam temperature is increased, the sensible heat that is added to the gasifier also increases which means that less char needs to be combusted to keep the combustion reactor at a specific temperature hence more char is available for the gasification reaction. According to char gasification and boundouard reactions, an increase in char feed to the gasifier will shift an equilibrium position forward leading to the formation of more H₂ and CO. On the contrary, more CO₂ will be consumed by an increase in char during the boundouard reaction hence the 22,77 % decrease in CO₂.

Syngas LHV for steam reforming of Wood Chips decreases from 13,03 to 10,40 MJ/Nm³ and this is attributed to a drop in CH₄ which has most weight on LHV. On the other hand CGE increases by 10,95 % and this is attributed to more char being gasified as steam temperature increases which leads to an increase syngas yield. The syngas yield increases by 0,49 Nm³/kg over the steam temperature range of 150 -1 000 °C.

As shown on figure 4-3, the same trend that is observed for Wood Chips is also observed for Rice Husk, the reason is the same as that provided above. Surprisingly, the behaviour for Sugarcane Bagasse is different, as shown on figure 4-2 as steam temperature is increased from 150 – 1000 °C, there is little

change in syngas composition, syngas LHV and CGE. As a result of this, it is not recommended to heat steam to high temperatures for the case of Sugarcane Bagasse gasification since the cost of operating and maintaining high temperature boilers is high.

Based on the trend observed on figure 4-1 and figure 4-3, the optimal steam temperature for steam reforming of Wood Chips and Rice Husk is 750 °C and 800 °C since beyond this temperature there is little change in the syngas composition. The composition at optimal steam temperature for Wood Chips feedstock is 53,22 %, 27,02 %, 15,12 %, 4,59 % and 0,05 % for H₂, CO, CO₂, CH₄ and N₂, respectively. Likewise, the composition at optimal steam temperature for Rice Husk feedstock is 47,11 %, 20,45 %, 21,41 %, 10,97 % and 0,06 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

5.1.2 Effect of Steam Temperature on LHV

Figure 4-4 shows the influence of steam temperature on the LHV of syngas for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks. It is observed that the LHV of syngas decrease with an increase in steam temperature for all 3 feedstock. As steam temperature is increased from 150 – 1000 °C the LHV of syngas decrease from 13,03 to 10,40 MJ/Nm³ for Wood Chips feedstock, from 10,63 to 10,44 MJ/Nm³ for Sugarcane Bagasse feedstock and from 14,80 to 10,79 MJ/Nm³ for Rice Husk feedstock. The drop in LHV is due to a decrease in CH₄ which has a LHV of 35,81 MJ/Nm³ which is almost 3 times the LHV of H₂ and CO which is 10,79 and 12,62 MJ/Nm³, hence the LHV trends follows the trend for CH₄. The CH₄ drops by 18,60 %, 3,32 % and 26,29 % for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks respectively. At the optimal temperature of 750 °C for Wood Chips feedstock and 800 °C for Rice Husk feedstock, the LHV is 10, 80 MJ/Nm³ and 11, 59 MJ/Nm³, respectively. As discussed earlier, Sugarcane Bagasse steam reforming has weak dependence on steam temperature, the LHV drops by only a small margin which is 0,19 MJ/Nm³ from 10,63 MJ/Nm³ to 10,44 MJ/Nm³.

5.1.3 Effect of Steam Temperature on CGE

Figure 4-5 shows the effect of steam temperature on CGE, it is observed that as steam temperature increases from 150 – 1000 °C the CGE increase by 10,95 %, 3,33 % and 11,68 % for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks, respectively. As shown by equation 15, CGE is proportional to LHV of syngas and syngas yield. Figure 5-1 below, shows that the syngas yield increases as steam temperature increases. The amount by which syngas yield increases by is greater than the

decrease in syngas LHV hence the overall trend for CGE follows that of syngas yield. The syngas yield increase by 43,03 %, 5,51 % and 58,77 % while LHV decrease by 20,17 %, 1,78 % and 27,11 % for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks, respectively. Technically, the increase in CGE is attributed to more char being gasified as steam temperature increases which leads to an increase in syngas yield.

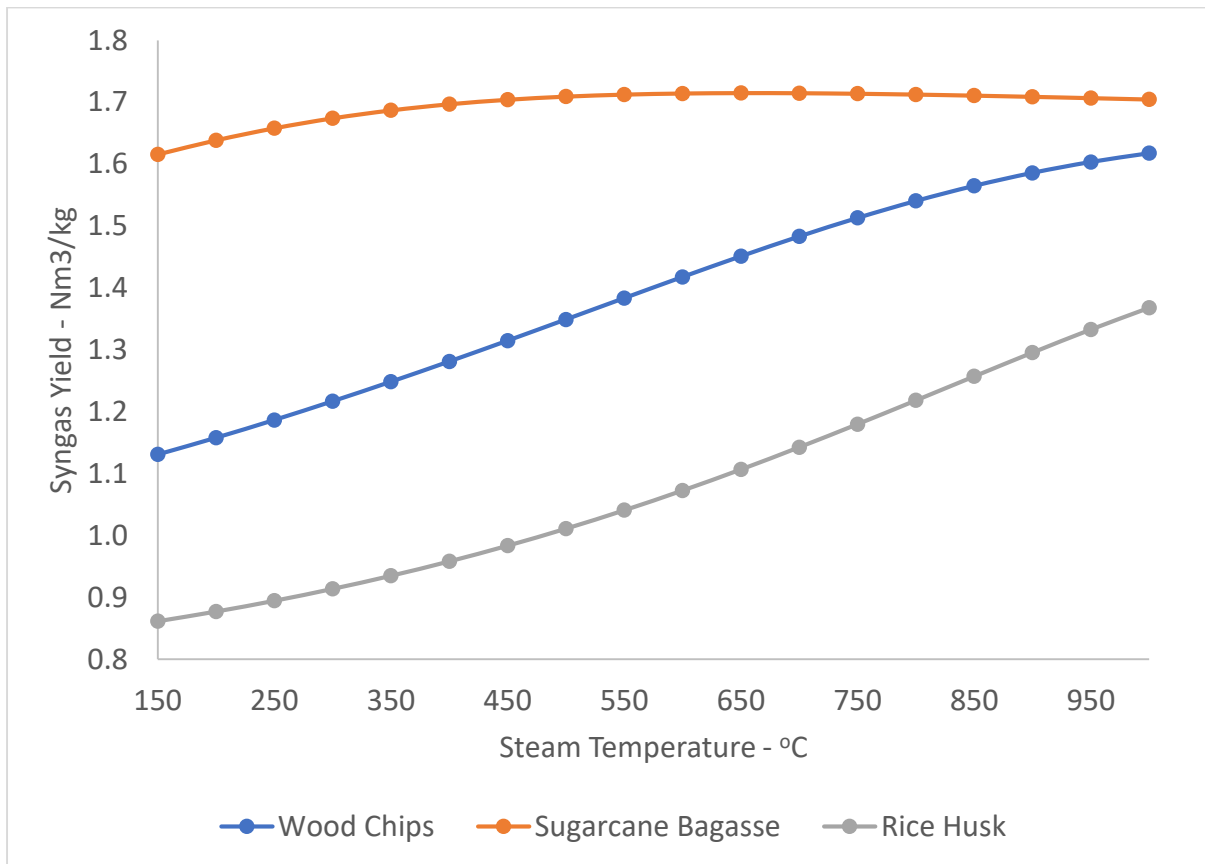


Figure 5-1: Effect of steam temperature on syngas yield for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

At optimal steam temperature of 750 °C and 800 °C for Wood Chips and Rice Husk steam reforming, the optimal CGE is 85,58 % and 82,31 %, respectively. For the case of Sugarcane Bagasse reforming, the CGE was found to be weakly dependent on steam temperature. Throughout the steam temperature range of 150 °C – 1000 °C the CGE was 91,80 % – 95,13 % which represents only a marginal increase of 3,33 %.

5.2 Gasifier Temperature

5.2.1 Effect of Gasifier Temperature on Syngas Composition

Figure 4-6 shows that the gasifier temperature has a significant impact on syngas composition for Wood Chips feedstock. Over the range 700 – 1 000 °C, both H₂ and CO increases. H₂ increase by 40,58 % and CO increase by 25,57 % points respectively. On the contrary, both CO₂ and CH₄ decrease. CO₂ decrease by 28,36 % while CH₄ decrease by 37,76 % points. N₂ decrease from 0,08 to 0,05 %.

The explanation for an increase in H₂ and CO is that since the char gasification, steam reforming and boudouard reaction are endothermic reactions. According to Le Chatelier's principle an increase in gasification temperature will shift the equilibrium point forward which will lead to the formation of more products which are CO and H₂ as well as a decrease in reactants. In the boudouard reaction, the reactant CO₂ is consumed as equilibrium point shift forward, this explains why CO₂ decreases when the gasification temperature is increased. Likewise, methane decomposition reaction is an endothermic reaction and an increase in gasifier temperature shift the equilibrium point forward thereby increasing H₂ generation and CH₄ consumption which explains why CH₄ decrease as gasifier temperature is increased from 150 – 1000 °C.

Since the water gas shift reaction is exothermic an increase in temperature with shift the equilibrium point to the left were one would expect CO₂ and H₂ to decrease and CO to increase. The reason this is not the case is that the heat of reaction for water gas shift reaction is 41,2 kJ/mol which is smaller than the combined heat of reaction for the endothermic reactions which are char gasification, boudouard, methane decomposition and steam reforming which are 131 kJ/mol, 172 kJ/mol and 74,8 kJ/mol, respectively.

Based on the trend observed on figure 4-6, the optimal gasifier temperature is 867 °C since beyond this point there is little change in the syngas composition. The composition at optimal gasifier temperature is 46,17 %, 21,00 %, 21,19 %, 11,58 % and 0,06 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

The same trend is observed on figures 4-7 and figure 4-8 for both Sugarcane Bagasse feedstock and Rice Husk feedstock as is for Wood Chips feedstock. The optimal gasifier temperature for Sugarcane Bagasse feedstock is 923 °C and the corresponding syngas composition is 52,62 %, 27,65 %, 14,92 %, 4,77 % and 0,05 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

For Rice Husk feedstock, the optimal gasifier temperature is observed to be 929 °C with the corresponding syngas composition of 55,26 %, 25,82 %, 15,51 %, 3,35 % and 0,05 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

5.2.2 Effect of Gasifier Temperature on Syngas LHV

The effect of gasifier temperature on LHV of syngas is shown on figure 4-9. It can be seen that as the gasifier temperature increase from 700 – 1 000 °C, the LHV of syngas drops from 16,12 to 9,37 MJ/Nm³ for Wood Chips feedstock, from 16,65 MJ/Nm³ to 10,33 MJ/Nm³ for Sugarcane Bagasse feedstock and from 15,62 to 10,07 MJ/Nm³ for Rice Husk feedstock. As discussed earlier, as the gasifier temperature increase, CH₄ drops by 37,76 % for Wood Chips feedstock, 40,80 % for Sugarcane Bagasse feedstock and 38,54 % for Rice Husk feedstock. According to Le Chatelier's principle, this is a result of the equilibrium point for the endothermic methane decomposition reaction shifting forward thus consuming more CH₄. Since the LHV of CH₄ is 35,81 MJ/Nm³ which is almost 3 times the LHV of H₂ and CO which is 10,79 and 12,62 MJ/Nm³, respectively, the LHV trends follows the trend for CH₄. At the optimal gasifier temperature of 867 °C for Wood Chips feedstock, the corresponding LHV is 11,78 MJ/Nm³. Similarly, at the optimal gasifier temperature of 923 °C for Sugarcane Bagasse feedstock, the corresponding LHV is 10,88 MJ/Nm³. Lastly, the optimal gasifier temperature of 929 °C for Rice Husk feedstock, the corresponding LHV is 10,42 MJ/Nm³.

5.3.3 Effect of Gasifier Temperature on CGE

The effect of gasifier temperature on CGE is shown on figure 4-10. It can be seen that as the gasifier temperature increase from 700 – 1 000 °C, the CGE increase from 71,38 % to 45,39 % at 924 °C before dropping to 83,58 % at 1 000 °C during gasification of Wood Chips. Similarly, the CGE increase from 73,37 % to 84,12 % at 974 °C before dropping to 83,58 % at 1 000 °C during gasification of Rice Husk. The peak CGE value reached at 924 °C and 974 °C during gasification of Wood Chips and Rice Husk, respectively corresponds to the peak value reached on the respective syngas yield trend as shown on figure 5-2. This is logical since CGE is proportional to syngas yield according to equation 15.

CGE is proportional to syngas yield and LHV. Figure 4-10 show that the CGE trend is similar to that of syngas yield which indicates that syngas yield has stronger impact on CGE for steam reforming of

Wood Chips and Rice Husk than LHV. In the case of Sugarcane Bagasse, the CGE increase as gasifier temperature is increased after a small initial drop of 0,77 % between 700 – 731 °C.

On the contrary, the trend for CGE for Sugarcane Bagasse steam reforming is different. The CGE increase as gasifier temperature is increased follows after a small initial drop of 0,77 % in CGE between 700 – 759 °C. After this initial period, as the gasifier temperature increases from 700 – 759 °C, the CGE decreases from 84,32 % to 83,79 %. As can be seen on figure 5-2, over the same temperature range, the syngas yield is nearly constant at 0,99 Nm³/kg while LHV decreases from 16,65 MJ/Nm³, to 14,97 MJ/Nm³, hence the overall effect is that CGE also decreases since it is proportional to the product of syngas yield and LHV. From gasifier temperature of 759 to 1 000 °C, the CGE increase sharply from 83,79 % to 94,16 % due to an increase in both LHV and syngas yield.

At the optimal gasifier temperature of 867 °C for Wood Chips feedstock, the corresponding CGE is 81,12 %. Similarly, at the optimal gasifier temperature of 923 °C for Sugarcane Bagasse feedstock, the corresponding CGE is 92,74 %. Lastly, the optimal gasifier temperature of 929 °C for Rice Husk feedstock, the corresponding CGE is 83,55 %.

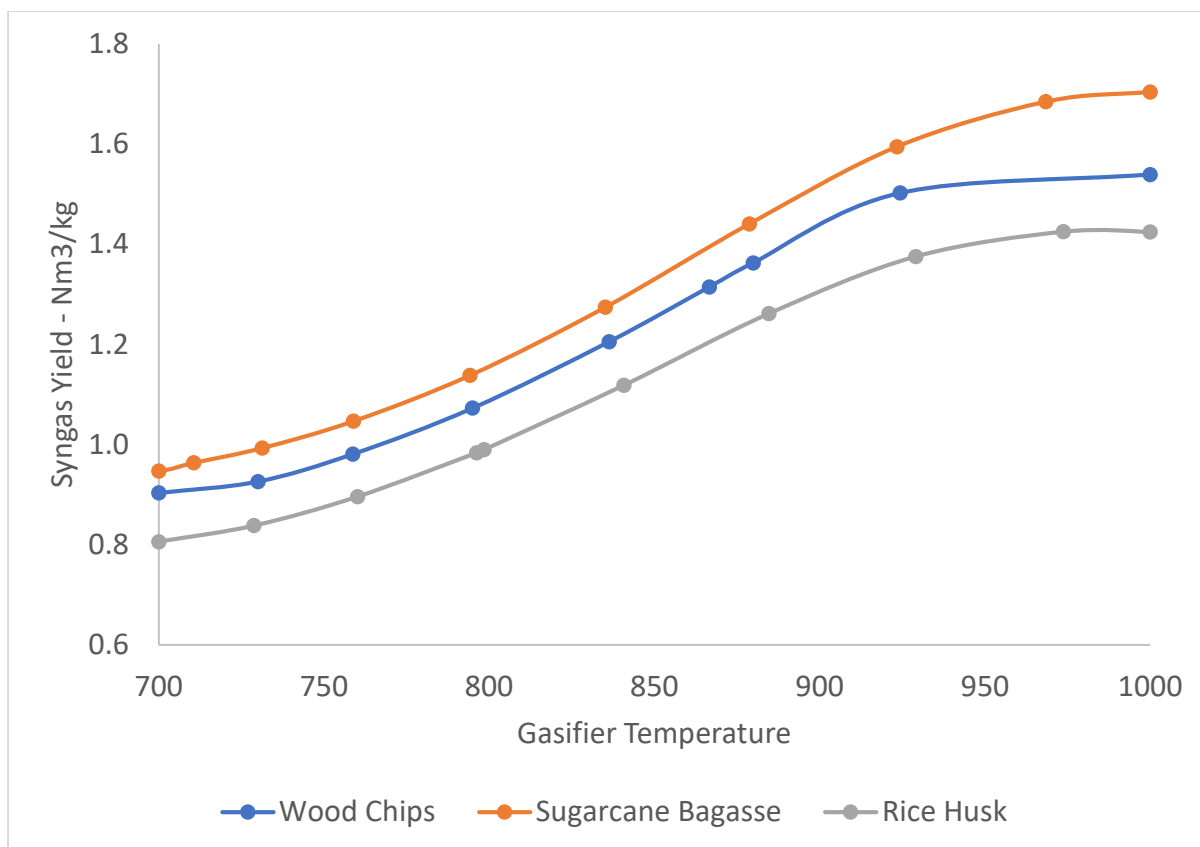


Figure 5-2: Effect of gasifier temperature on syngas yield for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

5.3 Steam to Feed Ratio

5.3.1 Effect of Steam to Feed Ratio on Syngas Composition

Figure 4-11, 4-12 and 4-13 shows that the steam to feed ratio has an impact on syngas composition produced from steam reforming of Wood Chips, Sugarcane Bagasse and Rice Husk. As steam to feed ratio increase from 0,4 – 1,0, Both H₂ and CO₂ increase while CO decrease significantly for all three feedstock, namely Wood Chips, Sugarcane Bagasse and Rice Husk.

H₂ increase only slightly by 5,94 % , 4,16 % and 9,39 % for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks, respectively. Similarly, CO₂ increase by 10,22 % , 10,75 % , and 4,97 % for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks, respectively. CO decrease by 15,39 % , 15,58 % and 9,41 % for Wood Chips, Sugarcane Bagasse and Rice Husk, respectively. CH₄ decrease by 4,94 % for Rice Husk while it remains almost unchanged for both Wood Chips and Sugarcane Bagasse.

Water is a reactant in three reactions that occur during gasification process which are char gasification (reaction 26), steam reforming (reaction 28) and water gas shift reaction (reaction 29). So, if steam to feed ratio increase, the amount of water in the reactants also increases, given that all other reactants are held constant. According to Le Chatelier's principle an increase in the concentration of reactants leads to the equilibrium point shifting forward forming more products which in the case of char gasification and steam reforming reactions are CO and H₂. In the case of water gas shift reaction the products are CO₂ and H₂.

An increase in CO from steam reforming reaction and H₂O from increasing steam to feed ratio leads to an increase in CO₂ generated by the water gas shift reaction due to an equilibrium point shifting forward which then explains why CO decrease and CO₂ increase during gasification of all three feedstocks namely, Wood Chips, Sugarcane Bagasse and Rice Husk.

Since CO decrease while H₂ decrease by only a small margin over the range of steam to feed ratio of 0,5 – 1,0, the optimum value of steam to feed ratio will be determined by the end use of the produced syngas. If the end use of the produced syngas is industrial chemical production where a low H₂/CO ratio ~ 2 is required, then the optimal steam to feed ratio would be 0,56, 0,72 and 0,43 for Wood Chips, Sugarcane Bagasse and Rice Husk, respectively.

However, if the end use of the produced syngas is hydrogen production, then the steam to feed ratio of 1,0 would be optimal since it would give the highest H₂/CO ratio of 3,90 and 6,0 for Wood Chips and Rice Husk, respectively. For sugarcane bagasse gasification, the highest H₂/CO ratio which occurs at steam to feed ratio of 1,0 is 2,69 which leads to the conclusion than syngas produced from Sugarcane Bagasse gasification is only suitable for industrial chemical production and not pure hydrogen. The effect of steam to feed ratio on H₂/CO for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks is shown on figure 5-3 below.

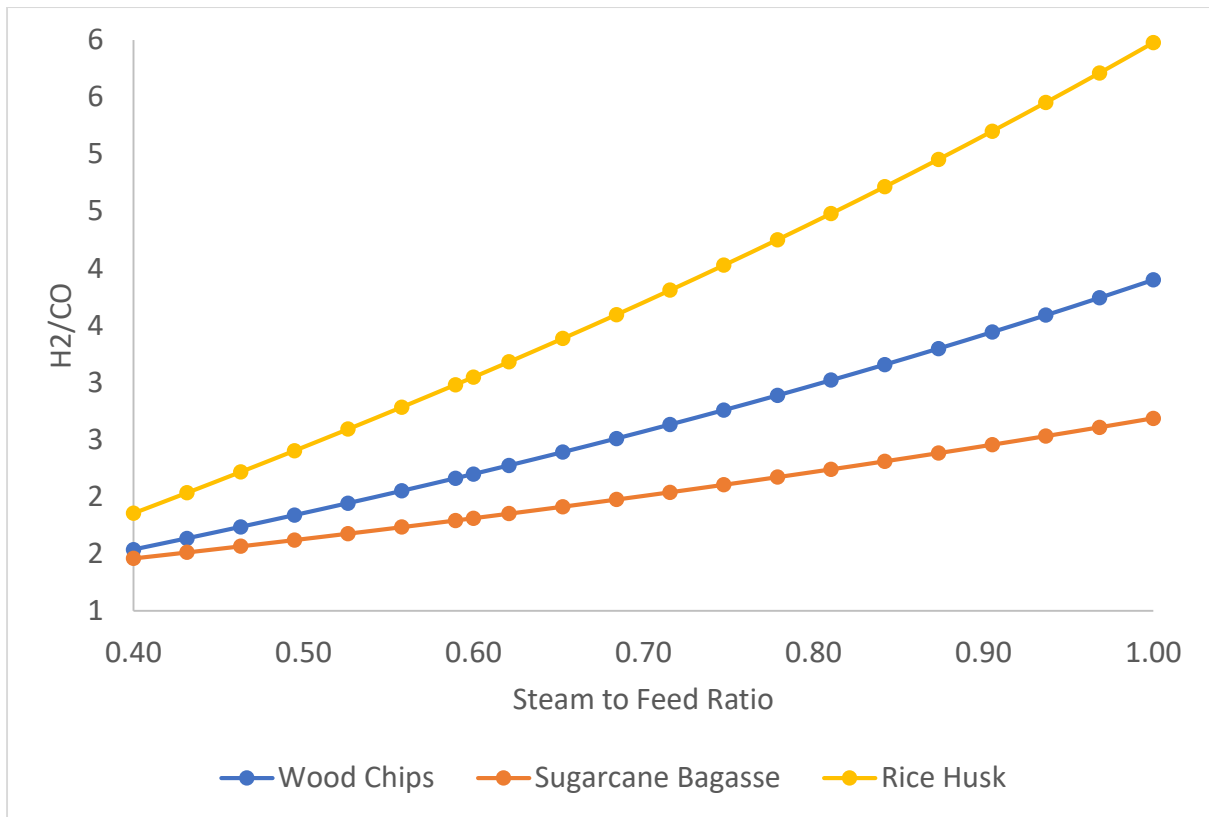


Figure 5-3: Effect of steam to feed ratio on H₂/CO ratio of syngas for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

5.3.2 Effect of Steam to Feed Ratio on Syngas LHV

Figure 4-14 shows the influence of steam to feed ratio on the LHV of syngas for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks. It is observed that the LHV of syngas decrease with an increase in steam to feed ratio. As steam to feed ratio is increased from 0,4 – 1,0 the LHV of syngas decrease from 12,59 to 11,02 MJ/Nm³ for Wood Chips feedstock, from 10,88 to 9,6 MJ/Nm³ for Sugarcane Bagasse feedstock and from 14,42 to 12,48 MJ/Nm³ for Rice Husk feedstock. Referring to figures 4-11, 4-12 and 4-13 it can be seen that H₂ increase slightly by 5,94 % , 4,16 % and 9,39 % for Wood Chips , Sugarcane Bagasse and Rice Husk feedstock, respectively. Over the same steam to feed ratio CO decrease sharply compared to H₂, the amount it decrease by is 15,39 % , 15,58 % and 9,41 % for Wood Chips , Sugarcane Bagasse and Rice Husk feedstock, respectively.

Moreover, CH₄ decrease by 4,94 % for Rice Husk while it changes by only < 1 % for Wood Chips and Sugarcane Bagasse. Since the LHV of CO which decrease drastically is 12,62 MJ/Nm³ which is higher

than LHV of H_2 which is $10,79 \text{ MJ/Nm}^3$ the overall trend for LHV follows trend for CO. Since CO is decreasing as steam to feed ratio is increased from 0,4 – 1,0 due to it being consumed during the water gas shift reaction, the LHV of syngas also decrease. The percentage LHV change is 12,52 %, 11,74 %, and 13,48 % for Wood Chips, Sugarcane Bagasse and Rice Husk. The reason for the highest decrease in syngas LHV produced from Rice Husk steam reforming is that, in addition to a decrease in CO which has higher LHV compared to H_2 , there is also a 4,94 % decrease in CH_4 which has even higher LHV amongst other combustive substances in syngas.

5.3.3 Effect of Steam to Feed Ratio on CGE

Figure 4-15 shows the effect of steam to feed ratio on CGE, it is observed that the CGE decrease from 81,73 % to 79,80 % for Wood Chips feedstock, from 95,03 % to 92,38 % for Sugarcane Bagasse feedstock and from 76,85 % to 76,71 % for Rice Husk feedstock. As shown by equation 15, CGE is proportional to LHV of syngas and syngas yield. As discussed previously, the LHV of syngas decrease with an increase in steam to feed ratio due to a drop in CO which is due to it being consumed in the water gas shift reaction. Figure 5-4 show that for all three feedstock the increase in steam to feed ratio increase the syngas yield which is defined as normalised volume of gas generated per unit mass of feed. This is due to the equilibrium point shifting forward generating more product gas when amount of water in the reactants is increased while other reactants are held constant. The overall effect of this on CGE is that it decreases slight with an increase in steam to feed ratio. The difference in CGE between steam to feed ratio of 0,4 – 1, 0 is 1,94 % for Wood Chips feedstock, 2,65 % for Sugarcane Bagasse feedstock and 0,14 % for Rice Husk feedstock.

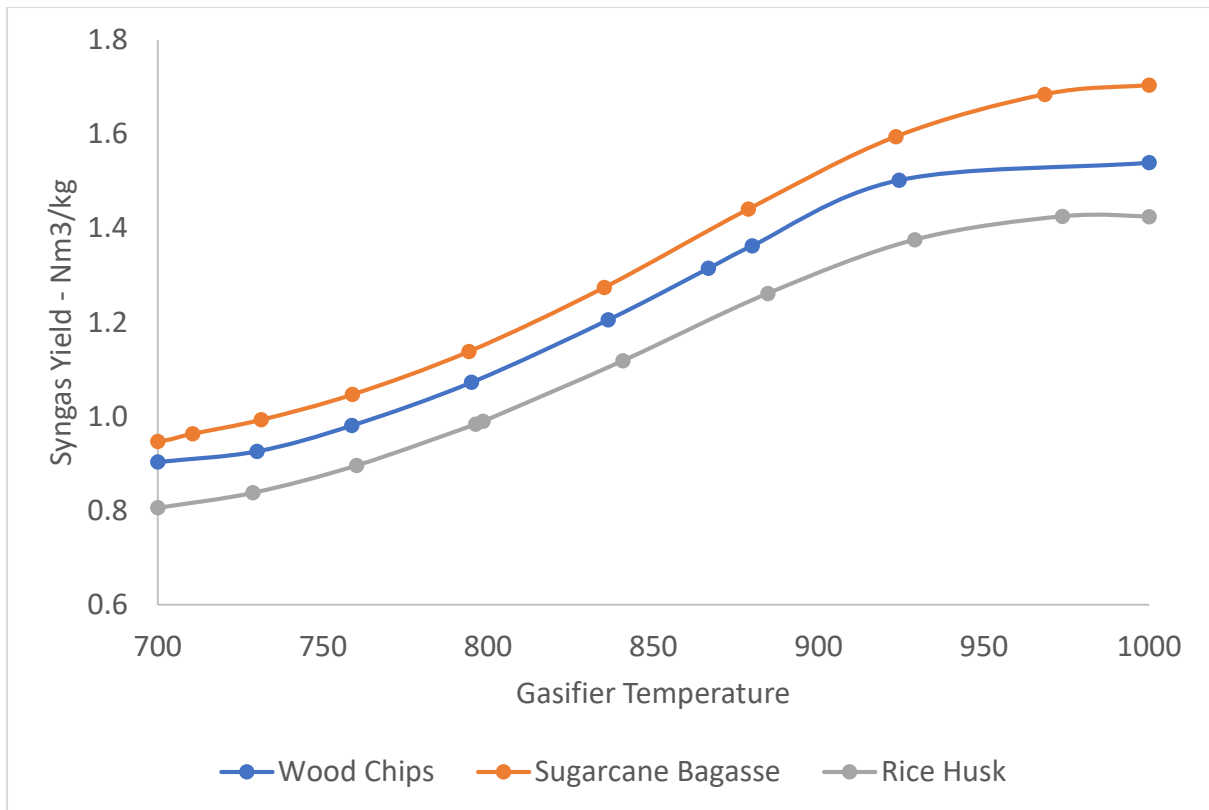


Figure 5-4: Effect of steam to feed ratio on syngas yield for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

5.4 Combustion Air Temperature

5.4.1 Effect of Combustion Air Temperature on Syngas Composition

Figure 4-16, shows that preheating combustion air has a huge impact on syngas composition for Wood Chips feedstock. As combustion air temperature is increased from 25 – 1000 °C, both H₂ and CO increases by 27,48 % and 22,22 %, respectively. On the contrary, both CO₂ and CH₄ decrease by 22,77 % and 26,91 %, respectively.

The explanation for this observation is that heating air which has specific heat capacity of 1,012 kJ/kg/K from 25 – 1000 °C increases the sensible heat added to the system by ~ 986,7 kJ/kg which means that less char needs to be combusted to keep the combustion reactor at a specific temperature hence more char is available for gasification reaction. According to char gasification and boundouard reactions, an increase in char feed to the gasifier will shift an equilibrium position forward leading to the formation of more H₂ and CO.

On the contrary, more CO₂ will be consumed by an increase in char during the boundouard reaction hence the 22,77 % decrease in CO₂. For this reason, it is recommended that combustion air be pre-heated. This can be achieved by installing a heat exchanger that can utilise exhaust gas from the combustion reactor as a heat source. Based on figure 4-16, the optimum combustion air temperature is 641 °C and the corresponding syngas composition is 52,29 %, 26,17 %, 15,96 %, 5,53 % and 0,05 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

The same trend that was observed for Wood Chips steam reforming was also observed for Sugarcane Bagasse and Rice Husk steam reforming as shown on figure 4-17 and 4-18. The optimum combustion air temperature for Sugarcane Bagasse as is for 641 °C Wood Chips steam reforming since beyond this point, the hydrogen yield start to show a small decline. At this temperature, the syngas composition is 56,93 %, 32,52 %, 10,27 %, 0,24 %, 0,04 % for H₂, CO, CO₂, CH₄ and N₂, respectively. For steam reforming of Rice Husk, the optimum combustion air temperature was found to be 898 °C. The syngas composition at this temperature is 52,39 %, 24,92 %, 16,89 %, 5,76 %, 0,05 % for H₂, CO, CO₂, CH₄ and N₂, respectively.

5.4.2 Effect of Combustion Air Temperature on Syngas LHV

The effect of combustion air temperature on LHV of syngas is shown on figure 4-19. It can be noted that as the combustion air temperature increase from 25 – 1 000 °C, the LHV of syngas drops from 14,20 to 10,33 MJ/Nm³ for Wood Chips feedstock, from 11,04 MJ/Nm³ to 10,44 MJ/Nm³ for Sugarcane Bagasse feedstock and from 15,61 to 10,53 MJ/Nm³ for Rice Husk feedstock. As discussed earlier, as the combustion air temperature increase, CH₄ drops by 26,91 % for Wood Chips feedstock, 6,36 % for Sugarcane Bagasse feedstock and 32,83 % for Rice Husk feedstock. Since the LHV of CH₄ is 35,81 MJ/Nm³ which is almost 3 times the LHV of H₂ and CO which is 10,79 and 12,62 MJ/Nm³, respectively, the LHV trends follows the trend for CH₄. At the optimal combustion air temperature of 641 °C for Wood Chips feedstock, the corresponding LHV is 10,93 MJ/Nm³. Similarly, at the optimal gasifier temperature of 641 °C for Sugarcane Bagasse feedstock, the corresponding LHV is 10,33 MJ/Nm³. Lastly, the optimal gasifier temperature of 897 °C for Rice Husk feedstock, the corresponding LHV is 10,86 MJ/Nm³.

5.4.3 Effect of Combustion Air Temperature on Syngas CGE

The effect of combustion air temperature on CGE is shown on figure 4-20. It can be seen that as the combustion air temperature increase from 25 – 1 000 °C , the CGE for steam reforming of all 3 feedstocks increased. The increases are 13,66 % , 5,52 % and 12,41 % for Wood Chips, Sugarcane Bagasse and Rice Husk. Even though, the syngas LHV for all 3 feedstocks shows at decline over the combustion air temperature range of 25 – 1 000 °C, the overall trend for CGE is upward which is due to the strong effect syngas yield has over the LHV. This can also be inferred from the slope of the LHV and syngas yield curves where it is noted that the upward slope on the syngas yield curve is steeper than the downward slope on the LHV curve. The trend for syngas yield is shown on figure 5-5 below:

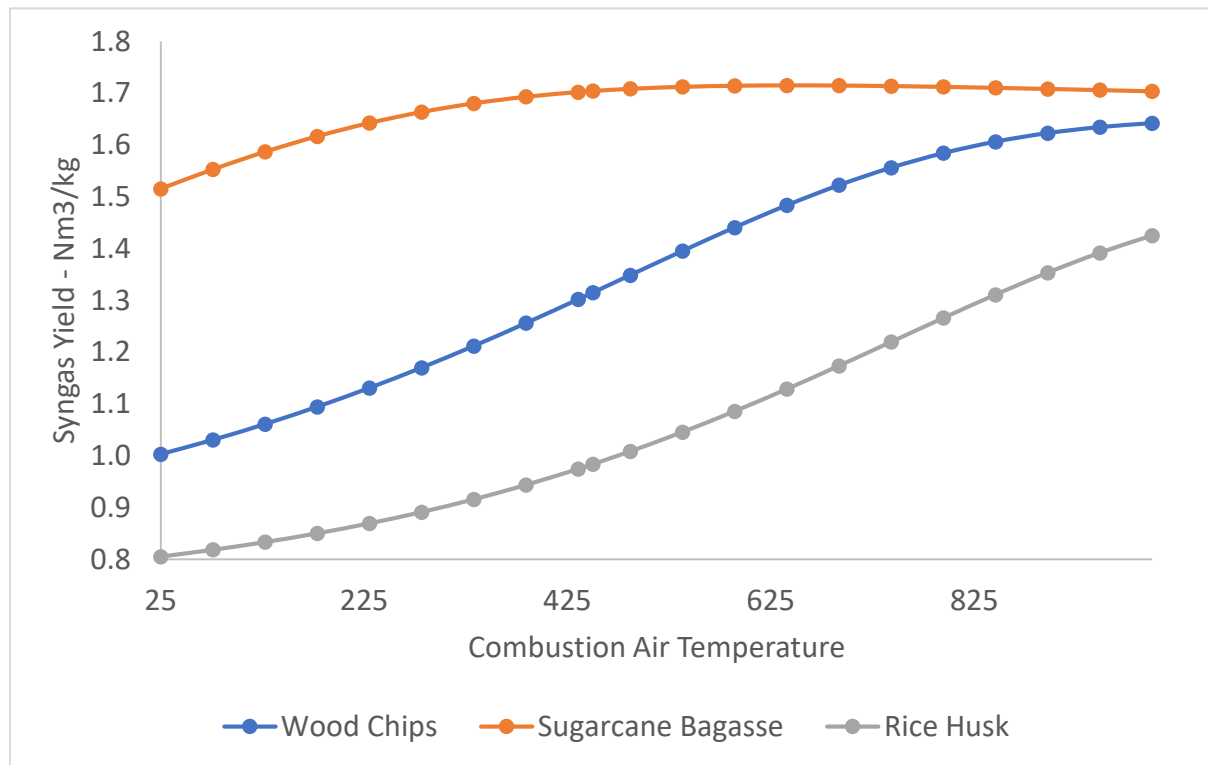


Figure 5-5: Effect of combustion air temperature on syngas yield for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

At the optimum combustion air temperature of 641 °C for Wood Chips and Sugarcane Bagasse feedstock, the corresponding CGE is 81,25 % and 91,71 % , respectively. Similarly, at the optimum combustion air temperature of 897,37 °C for Rice Husk feedstock, the corresponding CGE is 74,82 %.

5.5 Combustion Air to Feed Ratio

5.5.1 Effect of Combustion Air to Feed Ratio on Syngas Composition

The effect of combustion air to feed ratio (on mass basis) for Wood Chips steam reforming is shown on figure 4-21. As combustion air to feed ratio increase from 0,7 – 2,0, It was noted that both H₂ and CO decreases by 19,82 % and 15,23 %, respectively. On the contrary, CO₂ and CH₄ increase by 15,82 % and 19,21 %. The reason for a decrease in CO and an increase in CO₂ is that as combustion air to feed ratio increases, the combustion air available exceeds the stoichiometric required amount thereby leading to excess air. Excess air shifts the process towards complete combustion as opposed to gasification. It is well known that complete combustion produces CO₂ and H₂O.

Furthermore, as combustion air to feed ratio is increased, the amount of air flow reduces the temperature in the gasifier which then requires more char to be burnt to keep the gasifier temperature at the required level. When more char is burnt, there is less char available for gasification. According Le Chatelier's this change will shift the equilibrium for char gasification (reaction 26) backwards which leads to a reduction in H₂, hence the observed 19,82 % drop. Moreover, as complete combustion occur CO is converted to CO₂ which then leads to the equilibrium point on the water gas shift (reaction 29) moving backwards hence producing less H₂. The trend was observed for Sugarcane Bagasse on figure 4-22 and Rice Husk on figure 4-23.

Based on all the above considerations, combustion air to feed ratio needs to be as low as possible but high enough to allow complete char combustion to enable the gasifier temperature to be maintained. Based on the sensitivity analysis conducted in this research, the lowest combustion air to feed ratio is 0,7 and syngas composition for Wood Chips steam reforming is 52,54 %, 26,40 %, 15,73 %, 5,28 %, 0,05% for H₂, CO, CO₂, CH₄ and N₂ respectively. For Sugarcane Bagasse steam reforming, the composition at combustion air to feed ratio of 0,7 is 56,92 %, 32,88 %, 10,00 %, 0,16 %, 0,04% for H₂, CO, CO₂, CH₄ and N₂, respectively. Lastly, for Rice Husk steam reforming, the composition at combustion air to feed ratio of 0,7 is 41,99 %, 16,48 %, 25,53 %, 15,95 %, 0,07% for H₂, CO, CO₂, CH₄ and N₂, respectively. These are composition represent optimal conditions.

5.5.2 Effect of Combustion Air to Feed Ratio on Syngas LHV

The effect of combustion air to feed ratio on LHV of syngas is shown on figure 4-24. It can be noted that as the combustion air to feed ratio increase from 0,7 – 2,0 , the LHV of syngas increases from 10,89 MJ/Nm³ to 13,71 MJ/Nm³ for Wood Chips feedstock, from 10,35 MJ/Nm³ to 11,08 MJ/Nm³ for Sugarcane Bagasse feedstock and from 12,32 to 15,05 MJ/Nm³ for Rice Husk feedstock. As discussed earlier, as the combustion air to feed ratio increase, both H₂ and CO for all 3 feed stocks decreases due to a shift to complete combustion. Since LHV is a weighted average of LHV of individual combustible components in the syngas its trends follow that of H₂ and CO. At the optimal combustion air to feed ratio of 0,7 for Wood Chips, Sugarcane Bagasse and Rice Husk feedstock, the corresponding LHV is 10,89 MJ/Nm³, 10,35 MJ/Nm³ and 12,32 MJ/Nm³, respectively.

5.5.3 Effect of Combustion Air to Feed Ratio on Syngas CGE

The effect of combustion air to feed ratio on CGE is shown on figure 4-25. It can be seen that as the combustion air to feed ratio increase from 0,7 – 2,0 , the CGE for steam reforming of all 3 feedstocks analysed decreased. The amount they decrease by is 9,11 % , 5,46 % and 5,04 % for Wood Chips, Sugarcane Bagasse and Rice Husk. This is due to the reduction in the amount of char that is gasified which leads to a decrease in syngas yield. Figure 5-6, shows that as combustion air to feed ratio increase from 0,7 – 2,0 the syngas yield for all 3 feed stocks decreases.

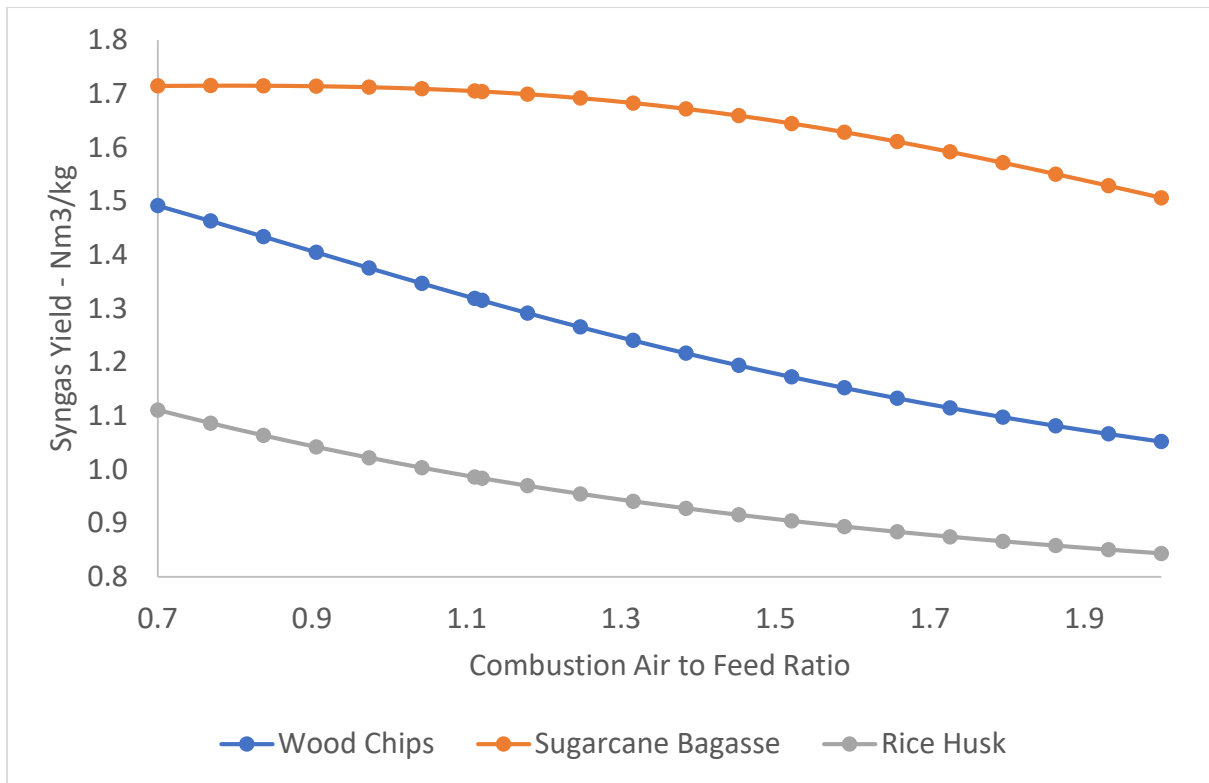


Figure 5-6: Effect of combustion air to feed ratio on syngas yield for Wood Chips, Sugarcane Bagasse and Rice Husk feedstocks

The optimal CGE at combustion air to feed ratio of 0,7 is 81,41 %, 91,82 % and 69,67 % for Wood Chips, Sugarcane Bagasse and Rice Husk, respectively.

Chapter 6 Conclusions and Recommendations

A simulation model for steam reforming of 15 different feedstock was developed using ASPEN Plus V 11. The model was successfully validated by comparing the model's results to experimental data for Wood Chips. The effect of varying steam temperature, gasifier temperature, steam to feed ratio, combustion air temperature and combustion air to feed ratio on syngas composition, syngas LHV and CGE was studied by utilising the sensitivity analysis tool on ASPEN Plus V 11.

The model results showed that the syngas from steam reforming of Wood Chips, Sugarcane Bagasse, Black Liquor and Pig Manure has a H_2/CO ratio of 1,81 – 2,20 which is ideal for the Fischer-Tropsch synthesis. The model results also showed that Food Waste, Municipal Solid Waste, Waste Plastics (PP), Waste Plastics (PE), Waste Tyres and Coal produced syngas with the poorest quality which makes them unsuitable for use in the chemical industry, however due to high LHV they are suitable for use in energy applications such as Combined Heat and Power (CHP) and Integrated Gasification Combined Cycle (IGCC).

The sensitivity analysis results indicated that increasing steam temperature improved syngas quality for Wood Chips and Rice Husk, however, there was little impact for Sugarcane Bagasse. The optimal steam temperature for steam reforming of Wood Chips and Rice Husk is 750 °C and 800 °C, respectively. Furthermore, sensitivity analysis indicated that increasing steam to feed ratio has good impact on hydrogen yield. As steam to feed is increased, both syngas LHV and CGE drops for Wood Chips, Sugarcane Bagasse and Rice Husk. In order to produce syngas with H_2/CO ratio of ~ 2, the optimal steam to feed ratio is 0,56, 0,72, and 0,43 for Wood Chips, Sugarcane Bagasse and Rice Husk, respectively.

To go further, sensitivity analysis indicated that both the gasifier temperature and combustion air temperature has a positive impact on syngas composition. In addition, the syngas LHV drops while CGE increase. The optimal gasifier temperature is 867 °C, 923 °C, and 929 °C while the optimal optimal combustion air temperature is 641 °C, 641 °C, and 898 °C for Wood Chips, Sugarcane Bagasse and Rice Husk steam reforming, respectively. Combustion air to feed ratio has a negative impact on syngas, so it should be kept as low as possible.

Based on the research conducted in this work, the follow future studies are recommended:

- ✓ Study on the steam reforming performance of a blend of different feedstock to understand if gasification result can be improving by blending different feedstocks.
- ✓ Compare the gasification result of the same feedstock using different technologies such as steam reforming, autothermal reforming, dry reforming to understand which technology produce best reforming results.
- ✓ Study on the effect of different gasification agents such steam, air, oxygen and carbon monoxide on syngas properties and on the gasification performance.
- ✓ Study on the impact of kinetic models as opposed to equilibrium model on syngas properties and on gasification performance.

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Appendices

Appendix A: Sensitivity Analysis for Wood Chips Steam Reforming

Table A-1: Sensitivity Analysis of Steam Temperature on Syngas Properties and Gasification Performance for Wood Chips Steam Reforming

Steam Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
150,00	37,41	14,33	28,14	20,05	0,07	1,13	13,03	77,17
200,00	38,88	15,38	27,03	18,65	0,06	1,16	12,82	77,73
250,00	40,36	16,47	25,88	17,23	0,06	1,19	12,60	78,34
300,00	41,84	17,59	24,71	15,79	0,06	1,22	12,39	78,99
350,00	43,31	18,73	23,53	14,37	0,06	1,25	12,18	79,67
400,00	44,76	19,87	22,36	12,96	0,06	1,28	11,98	80,39
450,00	46,17	21,00	21,19	11,58	0,06	1,31	11,78	81,12
500,00	47,54	22,12	20,05	10,24	0,05	1,35	11,59	81,88
550,00	48,84	23,21	18,95	8,95	0,05	1,38	11,40	82,65
600,00	50,08	24,25	17,89	7,73	0,05	1,42	11,23	83,41
650,00	51,23	25,24	16,90	6,59	0,05	1,45	11,07	84,16
700,00	52,28	26,16	15,97	5,54	0,05	1,48	10,93	84,89
750,00	53,22	27,02	15,12	4,59	0,05	1,51	10,80	85,58
800,00	54,06	27,80	14,34	3,75	0,05	1,54	10,68	86,21
850,00	54,77	28,51	13,65	3,02	0,05	1,56	10,59	86,79
900,00	55,37	29,14	13,05	2,39	0,05	1,59	10,51	87,30
950,00	55,86	29,70	12,52	1,87	0,05	1,60	10,45	87,74
1000,00	56,25	30,20	12,06	1,45	0,05	1,62	10,40	88,11

Table A-2: Sensitivity Analysis of Gasifier Temperature on Syngas Properties and Gasification Performance for Wood Chips Steam Reforming

Gasifier Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
700,00	15,95	3,65	41,05	39,26	0,08	0,90	16,12	71,38
730,03	19,75	5,11	39,08	35,98	0,08	0,93	15,66	75,98
758,73	25,21	7,63	35,95	31,14	0,08	0,98	14,83	76,23
794,99	32,51	11,71	31,24	24,48	0,07	1,07	13,75	77,28
836,28	40,72	17,10	25,34	16,77	0,06	1,21	12,56	79,29
866,61	46,17	21,00	21,19	11,58	0,06	1,31	11,78	81,12
879,88	48,27	22,56	19,55	9,56	0,05	1,36	11,48	81,94
924,34	53,72	26,75	15,18	4,30	0,05	1,50	10,71	84,29
1000,00	56,53	29,22	12,69	1,51	0,05	1,54	9,37	82,76

Table A-3: Sensitivity Analysis of Steam to Feed Ratio on Syngas Properties and Gasification Performance for Wood Chips Steam Reforming

Steam to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,40	42,88	27,91	16,74	12,41	0,06	1,24	12,59	81,73
0,43	43,54	26,64	17,55	12,21	0,06	1,25	12,43	81,65
0,46	44,15	25,45	18,31	12,03	0,06	1,27	12,29	81,56
0,49	44,70	24,32	19,03	11,89	0,06	1,28	12,15	81,46
0,53	45,19	23,26	19,72	11,77	0,06	1,29	12,03	81,36
0,56	45,64	22,26	20,37	11,68	0,06	1,30	11,91	81,26
0,59	46,05	21,31	20,99	11,60	0,06	1,31	11,81	81,16
0,60	46,17	21,00	21,19	11,58	0,06	1,31	11,78	81,12
0,62	46,41	20,41	21,58	11,54	0,06	1,32	11,72	81,05
0,65	46,74	19,56	22,15	11,49	0,06	1,33	11,63	80,95
0,68	47,04	18,74	22,69	11,47	0,06	1,34	11,55	80,84
0,72	47,32	17,98	23,21	11,45	0,05	1,34	11,47	80,73
0,75	47,56	17,24	23,70	11,44	0,05	1,35	11,40	80,63
0,78	47,79	16,55	24,17	11,44	0,05	1,36	11,34	80,52
0,81	47,99	15,89	24,63	11,45	0,05	1,36	11,28	80,41
0,84	48,17	15,26	25,06	11,46	0,05	1,37	11,23	80,31
0,87	48,33	14,66	25,47	11,49	0,05	1,37	11,18	80,20
0,91	48,48	14,08	25,87	11,52	0,05	1,37	11,13	80,10
0,94	48,60	13,54	26,25	11,55	0,05	1,38	11,09	80,00
0,97	48,72	13,02	26,62	11,60	0,05	1,38	11,05	79,90
1,00	48,82	12,52	26,97	11,64	0,05	1,38	11,02	79,80

Table A-4: Sensitivity Analysis of Air Temperature on Syngas Properties and Gasification Performance for Wood Chips Steam Reforming

Air Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
25,00	29,42	9,15	33,80	27,56	0,07	1,00	14,20	71,37
76,32	31,31	10,28	32,53	25,81	0,07	1,03	13,92	71,88
127,63	33,28	11,53	31,16	23,96	0,07	1,06	13,63	72,47
178,95	35,32	12,88	29,69	22,04	0,07	1,09	13,33	73,12
230,26	37,40	14,32	28,15	20,06	0,07	1,13	13,03	73,83
281,58	39,50	15,84	26,55	18,05	0,06	1,17	12,73	74,62
332,89	41,59	17,40	24,91	16,04	0,06	1,21	12,43	75,48
384,21	43,64	18,99	23,26	14,05	0,06	1,26	12,14	76,39
435,53	45,63	20,57	21,64	12,11	0,06	1,30	11,85	77,35
450,00	46,17	21,00	21,19	11,58	0,06	1,31	11,78	77,63
486,84	47,52	22,10	20,07	10,26	0,05	1,35	11,59	78,34
538,16	49,27	23,57	18,58	8,53	0,05	1,40	11,34	79,33
589,47	50,87	24,93	17,20	6,94	0,05	1,44	11,12	80,31
640,79	52,29	26,17	15,96	5,53	0,05	1,48	10,93	81,24
692,11	53,51	27,28	14,86	4,31	0,05	1,52	10,76	82,09
743,42	54,52	28,25	13,90	3,28	0,05	1,56	10,62	82,85
794,74	55,32	29,09	13,10	2,45	0,05	1,58	10,52	83,50
846,05	55,94	29,80	12,43	1,79	0,05	1,61	10,44	84,03
897,37	56,39	30,41	11,87	1,29	0,05	1,62	10,38	84,45
948,68	56,70	30,93	11,41	0,92	0,05	1,63	10,35	84,78
1000,00	56,90	31,38	11,03	0,65	0,04	1,64	10,33	85,03

Table A-5: Sensitivity Analysis of Air to Feed Ratio on Syngas Properties and Gasification Performance for Wood Chips Steam Reforming

Air to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,70	52,54	26,40	15,73	5,28	0,05	1,49	10,89	81,41
0,77	51,62	25,58	16,55	6,20	0,05	1,46	11,02	80,79
0,84	50,64	24,73	17,41	7,18	0,05	1,43	11,15	80,16
0,91	49,61	23,85	18,29	8,19	0,05	1,40	11,30	79,53
0,97	48,54	22,95	19,20	9,25	0,05	1,38	11,45	78,91
1,04	47,44	22,04	20,13	10,33	0,05	1,35	11,60	78,30
1,11	46,32	21,13	21,06	11,43	0,06	1,32	11,76	77,71
1,12	46,17	21,00	21,19	11,58	0,06	1,31	11,78	77,63
1,18	45,20	20,22	22,00	12,53	0,06	1,29	11,92	77,14
1,25	44,07	19,32	22,92	13,63	0,06	1,27	12,08	76,59
1,32	42,94	18,44	23,83	14,73	0,06	1,24	12,23	76,07
1,38	41,83	17,58	24,72	15,81	0,06	1,22	12,39	75,58
1,45	40,72	16,75	25,59	16,88	0,06	1,19	12,55	75,12
1,52	39,63	15,93	26,44	17,93	0,06	1,17	12,71	74,68
1,59	38,57	15,15	27,27	18,95	0,06	1,15	12,86	74,26
1,66	37,52	14,41	28,06	19,95	0,07	1,13	13,01	73,88
1,73	36,51	13,70	28,82	20,91	0,07	1,11	13,16	73,52
1,79	35,52	13,02	29,55	21,85	0,07	1,10	13,30	73,18
1,86	34,56	12,37	30,25	22,76	0,07	1,08	13,44	72,86
1,93	33,63	11,75	30,91	23,64	0,07	1,07	13,58	72,57
2,00	32,73	11,17	31,55	24,48	0,07	1,05	13,71	72,30

Appendix B: Sensitivity Analysis for Sugarcane Bagasse Steam Reforming

Table A-6: Sensitivity Analysis of Steam Temperature on Syngas Properties and Gasification Performance for Sugarcane Bagasse Steam Reforming

Steam Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
150,00	54,28	28,27	14,05	3,35	0,05	1,62	10,63	91,80
200,00	54,92	28,92	13,42	2,70	0,04	1,64	10,54	92,36
250,00	55,45	29,50	12,86	2,14	0,04	1,66	10,47	92,85
300,00	55,88	30,02	12,38	1,68	0,04	1,67	10,42	93,27
350,00	56,21	30,49	11,96	1,30	0,04	1,69	10,38	93,63
400,00	56,47	30,90	11,59	1,00	0,04	1,70	10,35	93,92
450,00	56,66	31,27	11,26	0,76	0,04	1,70	10,33	94,16
500,00	56,78	31,61	10,98	0,58	0,04	1,71	10,32	94,36
550,00	56,87	31,93	10,73	0,43	0,04	1,71	10,32	94,51
600,00	56,91	32,22	10,50	0,33	0,04	1,71	10,32	94,64
650,00	56,93	32,50	10,29	0,24	0,04	1,71	10,33	94,74
700,00	56,92	32,76	10,09	0,18	0,04	1,71	10,34	94,83
750,00	56,90	33,01	9,91	0,14	0,04	1,71	10,35	94,90
800,00	56,87	33,25	9,74	0,10	0,04	1,71	10,37	94,96
850,00	56,83	33,48	9,57	0,08	0,04	1,71	10,38	95,01
900,00	56,78	33,71	9,41	0,06	0,04	1,71	10,40	95,05
950,00	56,72	33,94	9,25	0,04	0,04	1,71	10,42	95,09
1000,00	56,67	34,15	9,10	0,03	0,04	1,70	10,44	95,13

Table A-7: Sensitivity Analysis of Gasifier Temperature on Syngas Properties and Gasification Performance for Sugarcane Bagasse Steam Reforming

Gasifier Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
700,00	12,82	3,02	42,52	41,56	0,08	0,95	16,65	84,32
710,60	15,35	3,94	41,23	39,40	0,08	0,96	16,26	83,81
731,36	18,89	5,43	39,29	36,32	0,07	0,99	15,73	83,55
758,89	23,99	7,96	36,22	31,77	0,07	1,05	14,97	83,79
794,18	30,97	12,07	31,54	25,36	0,06	1,14	13,95	84,89
835,11	39,12	17,59	25,53	17,70	0,06	1,27	12,78	87,07
878,74	46,85	23,26	19,52	10,32	0,05	1,44	11,68	90,01
923,41	52,62	27,65	14,92	4,77	0,05	1,59	10,88	92,74
968,44	55,74	30,25	12,25	1,72	0,04	1,68	10,45	94,11
1000,00	56,66	31,28	11,26	0,76	0,04	1,70	10,33	94,16

Table A-8: Sensitivity Analysis of Steam to Feed Ratio on Syngas Properties and Gasification Performance for Sugarcane Bagasse Steam Reforming

Steam to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,40	54,78	37,52	7,00	0,66	0,05	1,63	10,88	95,03
0,43	55,12	36,45	7,73	0,66	0,04	1,65	10,78	94,90
0,46	55,44	35,41	8,44	0,67	0,04	1,66	10,69	94,76
0,49	55,75	34,40	9,12	0,68	0,04	1,67	10,60	94,63
0,53	56,04	33,43	9,79	0,70	0,04	1,68	10,52	94,49
0,56	56,31	32,48	10,44	0,73	0,04	1,69	10,44	94,35
0,59	56,57	31,57	11,06	0,75	0,04	1,70	10,36	94,21
0,60	56,66	31,27	11,26	0,76	0,04	1,70	10,33	94,16
0,62	56,82	30,69	11,67	0,78	0,04	1,71	10,28	94,07
0,65	57,05	29,83	12,26	0,81	0,04	1,72	10,21	93,93
0,68	57,28	29,00	12,83	0,85	0,04	1,73	10,14	93,79
0,72	57,49	28,20	13,38	0,88	0,04	1,74	10,08	93,65
0,75	57,69	27,42	13,92	0,92	0,04	1,75	10,02	93,51
0,78	57,88	26,66	14,45	0,97	0,04	1,75	9,96	93,36
0,81	58,06	25,93	14,96	1,01	0,04	1,76	9,90	93,22
0,84	58,23	25,22	15,46	1,06	0,04	1,77	9,84	93,08
0,87	58,39	24,52	15,94	1,11	0,04	1,78	9,79	92,94
0,91	58,54	23,85	16,41	1,16	0,04	1,78	9,74	92,80
0,94	58,68	23,20	16,87	1,21	0,04	1,79	9,69	92,66
0,97	58,82	22,56	17,32	1,27	0,04	1,79	9,65	92,52
1,00	58,94	21,94	17,75	1,32	0,04	1,80	9,60	92,38

Table A-9: Sensitivity Analysis of Air Temperature on Syngas Properties and Gasification Performance for Sugarcane Bagasse Steam Reforming

Air Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
25,00	51,26	25,50	16,81	6,39	0,05	1,52	11,04	86,57
76,32	52,43	26,54	15,77	5,22	0,05	1,55	10,88	87,41
127,63	53,45	27,47	14,84	4,20	0,05	1,59	10,74	88,18
178,95	54,31	28,30	14,02	3,32	0,05	1,62	10,62	88,88
230,26	55,02	29,04	13,31	2,59	0,04	1,64	10,53	89,49
281,58	55,60	29,68	12,70	1,98	0,04	1,66	10,45	90,01
332,89	56,04	30,24	12,18	1,50	0,04	1,68	10,40	90,44
384,21	56,37	30,73	11,74	1,12	0,04	1,69	10,36	90,79
435,53	56,60	31,16	11,36	0,83	0,04	1,70	10,34	91,07
450,00	56,66	31,27	11,26	0,76	0,04	1,70	10,33	91,14
486,84	56,76	31,55	11,04	0,61	0,04	1,71	10,32	91,29
538,16	56,86	31,90	10,75	0,45	0,04	1,71	10,32	91,47
589,47	56,91	32,22	10,50	0,33	0,04	1,71	10,32	91,60
640,79	56,93	32,52	10,27	0,24	0,04	1,71	10,33	91,71
692,11	56,92	32,80	10,06	0,17	0,04	1,71	10,34	91,80
743,42	56,90	33,06	9,87	0,13	0,04	1,71	10,36	91,87
794,74	56,86	33,32	9,69	0,09	0,04	1,71	10,37	91,92
846,05	56,81	33,56	9,51	0,07	0,04	1,71	10,39	91,97
897,37	56,76	33,80	9,35	0,05	0,04	1,71	10,41	92,02
948,68	56,70	34,03	9,19	0,04	0,04	1,71	10,43	92,06
1000,00	56,64	34,25	9,03	0,03	0,04	1,70	10,44	92,09

Table A-10: Sensitivity Analysis of Air to Feed on Syngas Properties and Gasification Performance for Sugarcane Bagasse Steam Reforming

Air to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,70	56,92	32,88	10,00	0,16	0,04	1,71	10,35	91,82
0,77	56,93	32,64	10,18	0,21	0,04	1,71	10,34	91,75
0,84	56,93	32,40	10,36	0,27	0,04	1,71	10,33	91,67
0,91	56,90	32,14	10,56	0,35	0,04	1,71	10,32	91,57
0,97	56,86	31,88	10,76	0,45	0,04	1,71	10,32	91,46
1,04	56,78	31,61	10,99	0,58	0,04	1,71	10,32	91,32
1,11	56,67	31,32	11,23	0,74	0,04	1,70	10,33	91,16
1,12	56,66	31,27	11,26	0,76	0,04	1,70	10,33	91,14
1,18	56,53	31,01	11,49	0,93	0,04	1,70	10,34	90,98
1,25	56,34	30,68	11,78	1,16	0,04	1,69	10,36	90,76
1,32	56,10	30,33	12,10	1,43	0,04	1,68	10,39	90,50
1,38	55,82	29,95	12,45	1,74	0,04	1,67	10,43	90,22
1,45	55,48	29,54	12,83	2,11	0,04	1,66	10,47	89,90
1,52	55,08	29,10	13,25	2,52	0,04	1,64	10,52	89,54
1,59	54,64	28,63	13,70	2,99	0,05	1,63	10,58	89,15
1,66	54,14	28,14	14,18	3,50	0,05	1,61	10,64	88,74
1,73	53,59	27,61	14,70	4,06	0,05	1,59	10,72	88,29
1,79	52,99	27,05	15,25	4,66	0,05	1,57	10,80	87,83
1,86	52,35	26,47	15,84	5,30	0,05	1,55	10,89	87,35
1,93	51,67	25,86	16,44	5,98	0,05	1,53	10,98	86,86
2,00	50,95	25,23	17,07	6,69	0,05	1,51	11,08	86,36

Appendix C: Sensitivity Analysis for Rice Husk Steam Reforming

Table A-11: Sensitivity Analysis of Steam Temperature on Syngas Properties and Gasification Performance for Rice Husk Steam Reforming

Steam Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
150,00	25,21	6,23	36,93	31,54	0,09	0,86	14,80	74,32
200,00	26,54	6,87	36,16	30,34	0,08	0,88	14,60	74,63
250,00	27,97	7,59	35,31	29,06	0,08	0,89	14,38	74,97
300,00	29,49	8,39	34,37	27,68	0,08	0,91	14,15	75,37
350,00	31,08	9,28	33,35	26,22	0,08	0,93	13,91	75,81
400,00	32,75	10,25	32,24	24,67	0,08	0,96	13,66	76,30
450,00	34,49	11,32	31,06	23,06	0,07	0,98	13,41	76,85
500,00	36,27	12,47	29,80	21,39	0,07	1,01	13,15	77,46
550,00	38,09	13,69	28,48	19,67	0,07	1,04	12,88	78,13
600,00	39,94	14,98	27,10	17,91	0,07	1,07	12,61	78,86
650,00	41,78	16,32	25,69	16,15	0,07	1,11	12,35	79,65
700,00	43,61	17,70	24,25	14,38	0,06	1,14	12,09	80,49
750,00	45,39	19,08	22,82	12,65	0,06	1,18	11,84	81,38
800,00	47,11	20,45	21,41	10,97	0,06	1,22	11,59	82,31
850,00	48,74	21,79	20,04	9,37	0,06	1,26	11,36	83,25
900,00	50,26	23,07	18,74	7,87	0,06	1,30	11,15	84,19
950,00	51,65	24,27	17,54	6,49	0,06	1,33	10,96	85,12
1000,00	52,90	25,37	16,43	5,25	0,05	1,37	10,79	86,00

Table A-12: Sensitivity Analysis of Gasifier Temperature on Syngas Properties and Gasification Performance for Rice Husk Steam Reforming

Gasifier Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
700,00	16,60	3,30	41,14	38,87	0,09	0,81	15,62	73,37
728,83	20,93	4,80	39,02	35,17	0,09	0,84	15,46	75,50
760,18	27,09	7,42	35,65	29,75	0,08	0,90	14,52	75,80
796,22	34,49	11,32	31,06	23,06	0,07	0,98	13,41	76,85
798,48	34,95	11,59	30,75	22,63	0,07	0,99	13,34	76,94
840,77	43,28	16,89	24,90	14,86	0,07	1,12	12,12	79,02
884,62	50,46	22,04	19,43	8,01	0,06	1,26	11,10	81,56
929,09	55,26	25,82	15,51	3,35	0,05	1,38	10,42	83,55
973,77	57,48	27,98	13,38	1,11	0,05	1,43	10,13	84,12
1000,00	58,13	29,14	12,35	0,33	0,05	1,42	10,07	83,58

Table A-13: Sensitivity Analysis of Steam to Feed Ratio on Syngas Properties and Gasification Performance for Rice Husk Steam Reforming

Steam to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,40	29,53	15,92	28,71	25,76	0,08	0,91	14,42	76,85
0,43	30,49	14,99	29,19	25,25	0,08	0,93	14,22	76,84
0,46	31,38	14,15	29,62	24,76	0,08	0,94	14,04	76,84
0,49	32,20	13,40	30,00	24,31	0,08	0,95	13,87	76,84
0,53	32,96	12,72	30,35	23,90	0,08	0,96	13,72	76,85
0,56	33,65	12,09	30,67	23,52	0,08	0,97	13,58	76,85
0,59	34,29	11,50	30,96	23,17	0,08	0,98	13,45	76,85
0,60	34,49	11,32	31,06	23,06	0,07	0,98	13,41	76,85
0,62	34,87	10,96	31,24	22,85	0,07	0,99	13,33	76,85
0,65	35,40	10,46	31,50	22,56	0,07	1,00	13,22	76,85
0,68	35,89	9,99	31,75	22,30	0,07	1,01	13,12	76,85
0,72	36,33	9,54	31,98	22,07	0,07	1,01	13,03	76,84
0,75	36,74	9,12	32,20	21,86	0,07	1,02	12,94	76,83
0,78	37,12	8,73	32,42	21,67	0,07	1,02	12,87	76,83
0,81	37,45	8,36	32,62	21,50	0,07	1,03	12,79	76,81
0,84	37,76	8,01	32,81	21,34	0,07	1,04	12,73	76,80
0,87	38,04	7,68	33,00	21,21	0,07	1,04	12,67	76,78
0,91	38,30	7,36	33,18	21,09	0,07	1,04	12,61	76,77
0,94	38,53	7,07	33,35	20,98	0,07	1,05	12,56	76,75
0,97	38,74	6,78	33,52	20,89	0,07	1,05	12,52	76,73
1,00	38,92	6,51	33,68	20,82	0,07	1,05	12,48	76,71

Table A-14: Sensitivity Analysis of Air Temperature on Syngas Properties and Gasification Performance for Rice Husk Steam Reforming

Air Temperature °C	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
25,00	19,96	4,04	39,74	36,16	0,09	0,81	15,61	64,01
76,32	21,25	4,53	39,09	35,04	0,09	0,82	15,41	64,22
127,63	22,65	5,10	38,35	33,81	0,09	0,83	15,20	64,46
178,95	24,19	5,77	37,51	32,45	0,09	0,85	14,96	64,74
230,26	25,87	6,54	36,55	30,95	0,08	0,87	14,70	65,06
281,58	27,69	7,44	35,48	29,31	0,08	0,89	14,42	65,44
332,89	29,63	8,47	34,27	27,54	0,08	0,92	14,13	65,88
384,21	31,70	9,63	32,94	25,65	0,08	0,94	13,82	66,39
435,53	33,86	10,93	31,49	23,65	0,08	0,97	13,50	66,97
450,00	34,49	11,32	31,06	23,06	0,07	0,98	13,41	67,15
486,84	36,10	12,35	29,93	21,55	0,07	1,01	13,17	67,63
538,16	38,37	13,88	28,27	19,40	0,07	1,05	12,84	68,36
589,47	40,65	15,50	26,55	17,23	0,07	1,09	12,51	69,17
640,79	42,90	17,16	24,81	15,06	0,07	1,13	12,19	70,04
692,11	45,09	18,84	23,06	12,94	0,06	1,17	11,88	70,97
743,42	47,17	20,50	21,36	10,92	0,06	1,22	11,59	71,94
794,74	49,10	22,08	19,74	9,02	0,06	1,27	11,32	72,92
846,05	50,85	23,56	18,24	7,29	0,06	1,31	11,07	73,89
897,37	52,39	24,92	16,89	5,76	0,05	1,35	10,86	74,82
948,68	53,70	26,12	15,69	4,43	0,05	1,39	10,68	75,67
1000,00	54,78	27,17	14,66	3,33	0,05	1,42	10,53	76,42

Table A-15: Sensitivity Analysis of Air to Feed Ratio on Syngas Properties and Gasification Performance for Rice Husk Steam Reforming

Air to Feed Ratio	H ₂ vol %	CO vol %	CO ₂ vol %	CH ₄ vol %	N ₂ vol %	Syngas Yield Nm ³ /kg	Syngas LHV kJ/Nm ³	CGE %
0,70	41,99	16,48	25,53	15,95	0,07	1,11	12,32	69,67
0,77	40,68	15,52	26,53	17,20	0,07	1,09	12,51	69,18
0,84	39,40	14,60	27,50	18,42	0,07	1,06	12,69	68,71
0,91	38,16	13,74	28,43	19,61	0,07	1,04	12,87	68,29
0,97	36,95	12,92	29,31	20,75	0,07	1,02	13,05	67,89
1,04	35,77	12,14	30,16	21,86	0,07	1,00	13,22	67,53
1,11	34,64	11,41	30,95	22,92	0,07	0,99	13,39	67,19
1,12	34,49	11,32	31,06	23,06	0,07	0,98	13,41	67,15
1,18	33,55	10,73	31,71	23,94	0,08	0,97	13,55	66,88
1,25	32,50	10,10	32,41	24,91	0,08	0,95	13,70	66,60
1,32	31,50	9,51	33,08	25,83	0,08	0,94	13,85	66,34
1,38	30,54	8,97	33,70	26,72	0,08	0,93	14,00	66,10
1,45	29,62	8,46	34,29	27,56	0,08	0,92	14,13	65,88
1,52	28,74	7,99	34,83	28,36	0,08	0,90	14,27	65,68
1,59	27,90	7,55	35,35	29,12	0,08	0,89	14,39	65,49
1,66	27,10	7,14	35,83	29,85	0,08	0,88	14,51	65,32
1,73	26,33	6,77	36,28	30,53	0,08	0,87	14,63	65,16
1,79	25,61	6,42	36,70	31,18	0,09	0,87	14,74	65,01
1,86	24,92	6,10	37,10	31,80	0,09	0,86	14,85	64,88
1,93	24,26	5,80	37,47	32,39	0,09	0,85	14,95	64,75
2,00	23,63	5,52	37,82	32,95	0,09	0,84	15,05	64,63