



**Process optimization of syngas production from
gasification of waste plastic using a small-scale
infrared reactor**

By:

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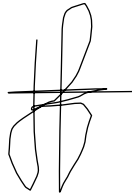
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Executive Summary

Due to the negative impact of fossil fuel on the environment and its finite potential, the quest for renewable energy sources, climate protection, energy sustainability, and conservation of humankind's natural habitat has become a contemporary civilization's greatest challenge. To achieve such a goal, governments, scientists, and engineers have to design ways to meet the world's energy security while addressing climate change and reducing the environmental pollution.

Currently, South Africa faces two major challenges, (i) energy security and (ii) environmental pollution, particularly the one caused by waste plastic. Despite the country's effort to mitigate these two serious challenges, it is clear in regard to the country's current energy crisis and environmental pollution that there is a need for a more drastic approach in solving these challenges. This work focuses on the optimization of syngas production from gasification of waste plastic using a small-scale IR reactor. The work is based on a modeling and simulation approach using Aspen plus®, and on experimental analysis of a pilot gasification plant.

A model was simulated on Aspen plus® and the kinetic free equilibrium model was used to investigate the optimization of waste plastic gasification. The gasification plant is a small laboratory scale plant that aims to generate gaseous products as fuel for further processing in a separate process outside the scope of this study. The gasification plant not only constitutes an infrared reactor, which is responsible for the gasification of the feedstock, but also of a catalytic water gas shift (WGS) system that is responsible for enhancing the hydrogen production via the concentration of syngas thermal energy. It was evident from this simulation study that the temperature at which syngas production was optimum was in the range 750–800°C. At this interval, the model revealed syngas content of 39% H₂, 32% CO, 17% CO₂, and 10% CH₄. Pertaining to the flow rate parameters, the water flow rate appears to generate more syngas when alternated in comparison to the airflow rate. The experimental studies did not agree with the simulation and modeling results. However, they were in agreement with the literature. At a temperature of 653°C, syngas produced was composed of 21.3% H₂, 5.7% CO, 15.2% CO₂ and 0.2% CH₄. The results obtained in this work particularly the hydrogen and

carbon monoxide content are highly desirable for the Fischer-Tropsch synthesis.

This thesis is dedicated to my late father Tadonkeng Jean-Marie (1939 – 1997) and my mother Tadonkeng Mawanba Nzeki Evodie Danielle and Tadonkeng Makougue Victorine. Your love, your hard work, your sacrifice, your encouragement, and your ever-ending belief in me and my dreams are the sources of inspiration and motivation.

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List of Symbols:

Alphabet Notation:

- A:** Surface area, m^2
- C_p:** Specific heat, $J/kg * K$
- F:** View factor
- k:** Thermal conductivity, $W/m * K$
- r:** Resistivity, $\Omega.m$
- T:** Temperature, ° C or K
- V:** Air velocity, m/s

Greeks Notation:

- ϕ:** Thermal diffusivity, m^2/s
- ρ:** Density, kg/m^3
- Σ:** Stephan–Boltzmann constant, $W/m^2 * K^4$
- ε:** Emissivity

Subscripts Identification:

- IR:** Infrared
- R:** Radiation
- s:** Surface or surrounding
- i:** Surface i
- ir:** Irradiation
- j:** Surface j
- h:** Heater

List of Abbreviations:

PE:	Polyethylene
PP:	Polypropylene
PS:	Polystyrene
PET:	Polyethylene terephthalate
HDPE:	High density polyethylene
LDPE:	Low density polyethylene
PVC:	Polyvinyl chloride
WtE:	Waste to Energy
CO:	Carbon monoxide
CO ₂ :	Carbon dioxide
O ₂ :	Oxygen
CH ₄ :	Methane
N ₂ :	Nitrogen
H ₂	Hydrogen
C:	Carbon
MSW:	Municipal Solid Waste
UNEP:	United Nations Environmental Program

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1. Chapter 1: Introduction

Current civilization development is almost dependent on fossil fuel energy. Energy is basic to fulfill all human being's needs. It enables productivity, prosperity, and comfort. Under the current status quo, the world's energy production is heavily reliant on fossil fuels. Nevertheless, concerning scientific evidence, human activities, and more especially fossil fuel combustion, is negatively changing the climate and the environment in ways that the well-being, evolution, and destiny of human society is currently under threat (Richardson *et al.*, 2009). Otherwise stated, one fundamental condition for human survival cannot be thought of without redesigning the present-based fossil-fuel energy systems towards a high share of renewable energy sources (Hake *et al.*, 2015).

In this regard, the quest for renewable energy sources, climate protection, energy sustainability, and conservation of humankind's natural habitat has become a contemporary civilization's greatest challenge (Bevan, 2012). To achieve such a goal, governments, scientists, and engineers have to design energy pathways that minimize the impact on the environment. The generation of energy from waste plastic provides a means to do this. Waste plastic can be treated and used as a source of energy generation either in the liquid form as fuels or the gas form as hydrogen and syngas (Guyemat & Adonis, 2012).

Syngas is also known as synthetic gas, can be used for several purposes and can be obtained from numerous processes and techniques. Nevertheless, with recent increases and awareness of environmental pollution, a huge industry has developed around the production of syngas from solid waste.

Recent studies (Getor *et al.*, 2020; Mai *et al.*, 2020; Tzatzadakis *et al.*, 2020) all agree that the global production of plastic has increased worldwide. This global plastic production growth means for most countries that there are an ever-increasing demand and consumption of plastics. Hence, the results of an increase in waste plastic generated by households and industries. This increase in waste plastic generation is creating more issues for waste disposal methods as plastic is not a biodegradable element and thus it constitutes a heavy pollutant for the environment.

Based on a study conducted by Dikgang et al (2012), approximately 8 billion plastic carrier bags are annually consumed in South Africa. Another study (Plastics SA, 2017) revealed that between 2013 and 2014, South Africans consumed 1.4 million tonnes of plastics. This is equivalent to an estimated amount of 1.6 % of the South African GDP. This value corresponds to approximately 14.2% of the country's manufacturing as depicted by Holtzhausen, (2017). Landfills are one of the major South African waste disposals routes. Consequently, the vast part of these plastics ends up in landfills. Even though Plastics SA (2017) reported that an estimated 32.9% of all plastics packaging is recovered through recycling, the challenge still remains. Indeed, many researchers (Anaraki 2012; Yanga et al., 2012) have established that due to the high contaminant content and other issues after recycling, plastics cannot be used for the application as previously used). The consumer application and the market for recycled plastics are very restrained. He et al., (2009) supported this view by indicating that another potential for plastic and particularly waste plastic is its viable energy source since it contains high energy density.

According to Wu & Williams (2010), the recent increase in research studies that treat waste plastic as an energy source is due to the growth in plastic consumption, the pollution it caused when disposed of in landfills or when incinerated, and finally its rich energy potential for electricity generation or petrochemicals feedstock.

1.1. Plastics

Plastics can be defined as a group of synthetic organic materials that can be classified based on their performance or composition and which are produced through polymerization. Besides polymers as part of their constituent, there are other substances present in their composition that increase the quality and/or significantly decrease the manufacturing costs. The selection of these polymers is based upon their high molecular mass which rendered them easy for molding or extrusion consequently can take any desired shapes. Thermosets and thermoplastics among many others are the most known two major groups of plastics (Mbourou & Adonis., 2016).

The growth of the plastics industry in the past 50 years (Getor, 2020) makes it one of the most lucrative industries. Nowadays, plastics are almost used every day and in all aspects of life as well as in almost any shape, form, and color. However, the population growth added to the plastics consumption increase led to an upsurge of waste plastics every year. Waste plastics packaging and products constitute an increasing quota of the solid waste stream in municipalities. Thermoplastics constitute the major portion of plastics found in the Municipal Solid Waste (MSW). Those thermoplastics are made majorly of Polyvinyl Chloride (PVC), Polystyrene (PS), Polypropylene (PP), and Polyethylene (PE) (Xiao et al., 2007; Toledo et al., 2011). Worldwide, thermoplastics represents two-thirds of plastics sales.

The MSW in general, and the waste plastics in particular, have several alternative techniques for treatment. The commonly known (Toledo et al., 2011) are mechanical recycling, incineration, chemical recycling, landfilling, and energy recovery.

1.1.1. Thermoplastics

Thermoplastics can be defined as polymers that become moldable and plastic either by melting or heating of crystal, and by exceeding the temperature of the glass alteration (Rennie, 1999). The most encountered thermoplastics are Polystyrene (PS), Polyethylene (PE), and Polyvinyl Chloride (PVC) Polypropylene (PP). Thermoplastics are known as plastics that soften during processing while the heat is applied and they would get hard when cooling. If reheated, thermoplastics can be turned into new plastic products that can be softened by repeatedly reheating them (UNEP, 2009).

1.1.2. Thermosets

The materials that are irreversibly set to any given form due to heating and/or chemical reactions they underwent are known as thermosets (Rennie, 1999). Thermosets are known as plastics that demonstrate a surge in flow-ability upon application of heat. They are also known as plastics that solidify at higher temperatures and remain at this state. Other characteristics of thermosets are their infusibility and insolubility. With regards to plastic recycling, even though policies are put in place by the South African government to encourage plastics re-

usage as inferred in Figure 1.1 below, it is still more than 87% of plastics that go to MSW landfill disposal. Furthermore, figure 1.1 also showcases that through the years from 2009 till 2014.

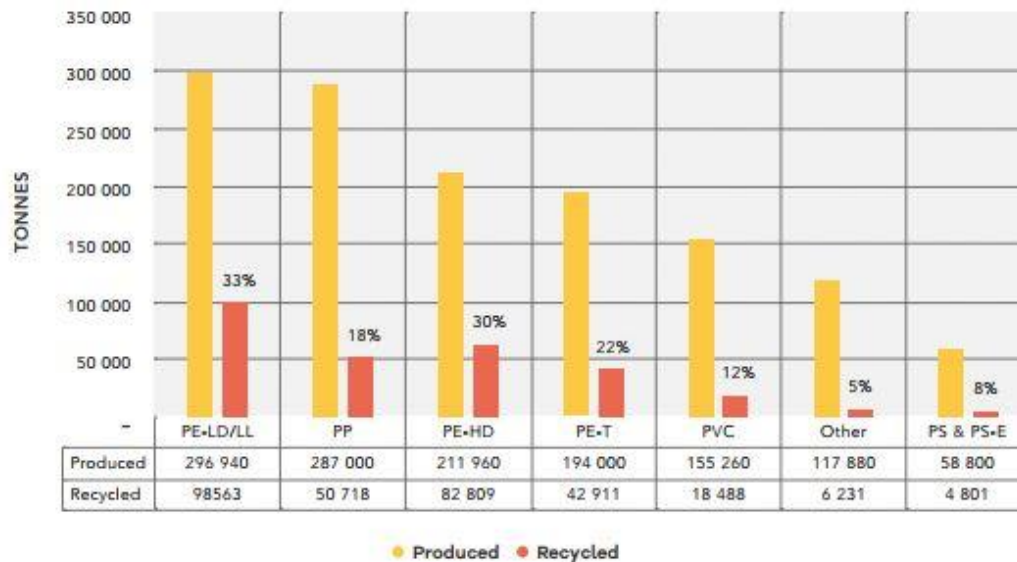


Figure 1-1: Plastic Production by polymer type versus recycling tonnes (Green Cape 2016)

1.1.3. Current Waste Plastics Treatment Methods

Shi et al., (2011) indicated that although it has been demonstrated that landfilling is advantageous to simple waste disposal in discharges, it still has many disadvantages. Among many other disadvantages that Shi et al., (2011) highlighted is the vast space or area occupied by landfilling. They also addressed the bad odor and greenhouse gas emissions caused by landfilling. The research work of Varadi et al. (2007) shows that the waste disposal technique or method nurtures serious health and pollution concerns added to the concerns with landfill site appearance Sharp and Ness (1991). Table 1.1 shows contemporary techniques of waste management and it further highlights the advantages and disadvantages of each waste management technique. Table 1.2 illustrates the number of landfill sites legally recognized by the South African government across each province. Eastern Cape, Gauteng, KwaZulu Natal, and Northern Cape provinces all have above 100 approved landfill sites. Gauteng and Eastern Cape provinces have the highest number (160 and 120 respectively) of approved landfill sites.

Tables 1.1 and 1.2 reflect on one hand the magnitude of landfill site problems and on the other hand, the urgency to explore alternatives means of waste management as the current treatment methods are proven to be full of limits.

Table 1-1: Waste Management Current Methods (Mbourou & Adonis, 2016)

Methods	Benefits	Drawbacks
Waste Incineration	Volume and weight reduced Immediate waste reduction Destruction in seconds Incineration can be done at generation site	The constant formation of furans and toxic dioxins
Waste Landfill	the cheapest method of disposal	Usually are situated in close vicinity to financially disadvantage Area and unofficial settlements Formation of greenhouse gas
Waste Recycling (Conventional)	Some Plastic materials are Reused	This process requires intensive labor The potential for polymer to lose its quality

Table 1-2: Landfill Sites according to South African province in 2010 (Africa, 2010)

Provinces	Approved landfill sites
Limpopo	44
Gauteng	160
Mpumalanga	72
North West	35
Eastern Cape	120
KwaZulu Natal	119
Free State	67
Northern Cape	103
Western Cape	97
South Africa	817

1.2. Significance of gasification in handling waste plastic

In regard to the huge increase in plastic waste, its high heat of combustion content, and its growing availability and accessibility even in rural areas, scientists and engineers believe that plastic waste could be a tremendous potential resource in energy generation and fuel in particular (Saeed, et al., 2009). The advantages of plastics over paper and wood are that plastics do not absorb much moisture. Furthermore, biomass water content is significantly higher than that of plastics. (UNEP, 2009).

When processing plastic waste into fuel, there are several properties that need to be taken into account as those properties influence the quality of the fuel. For instance, the type of plastics and the constituents of other waste which might be in the process. Moreover, in order to achieve an effective waste plastic to energy conversion, it is fundamental to take into account the type of technology involved in the conversion process. Indeed, during waste plastic conversion to energy, appropriate technology configuration is required. This last aforementioned property does not only focus on selection criteria like the area, the environment, the communities, the finances, and technical parameters but also on the feedstock to be processed. Consequently, for each type of waste plastic conversion technology, there is an adequate feedstock. According to the UNEP (2009) report, there is a higher degree of chance that feedstock with various types of plastic in their composition might contain substances that are a risk to humans and the environment. For instance, sulfur, halogens, nitrogen, or any other hazardous substances that are a danger to the environment and to humans. Apart from PVC which is reported nonefficient for energy generation when gasified; the use of gasification technology was proven to be efficient for non-recyclable plastics (Mbourou & Adonis 2016). Additionally, it reduces the amount of waste disposed to landfills (Cheng & Hu, 2010). Due to plastic high calorific values, plastic materials used as feedstock in the gasification process may be the solution in electricity generation for a cleaner and proper electricity distribution in households. The heating values of numerous kinds of solid fuel and wastes are summarized in Table, 1.3 (UNEP, 2009), and as it can be seen, plastics have a

typical heating value of 11.000kcal/kg. This means plastics have high energy potential.

Table 1-3: Different Fuel and waste Heating Values (UNEP, 2009)

Fuel of waste	Typical heating value in thousands (kcal/kg)
Coal	6-8
Refuse derived fuel	4-5
Refuse derived paper and plastic fuel	6-8
Heavy oil	9.5
Plastics (polyethylene)	11
Typical municipal waste	1-1.5
Wood/paper	4.3

1.3. Problem Statement

2.1 billion tonnes/ year of municipal solid waste (MSW) is generated globally and this amount is expected to grow to 3.40 billion by 2050 (Gourmelon, 2015). South Africa generates a total of 54.2 million tonnes of MSW yearly of which 4.47 million tonnes is plastic waste. MSW generation is associated with various problems such as soil and water contamination, air pollution, climate change, and several others. Despite the problems MSW is associated with, it can also be seen as a resource for energy generation especially in the current world context of the energy crisis. There are several methods to address the issues caused by MSW generation. With increasing awareness about environmental pollution and energy transition, the generation of syngas from waste plastic could position itself as a solution to both environmental and energy challenges. However, the current conversion of waste plastic into syngas is inefficient (Muhammad et al., 2021). Hence this study will investigate different process conditions and feed characteristics to optimize the syngas production through the gasification of waste plastic. This process would be conducted using a model and simulation generated from Aspen Plus.

1.4. Research Aims and Objectives

This present work aims to optimize the yield of syngas from waste plastic gasification using infrared radiation.

In order to achieve this, the following objectives will be investigated:

- To optimize the slow pyrolysis step of waste plastic gasification as a function of heating rate, temperature, and holding time through simulation.
- To simulate a predictive model for the evolution of volatiles during the pyrolysis reaction. A Gibbs model was used for this function.
- Investigate the effect of Pressure on the yield of syngas using Aspen.
- To improve the efficiency and the environmental performance of the gasification process through simulation using Aspen plus® software.
- To study the influence or impact of airflow rate and water flow rate on the yield of syngas from plastics pellets.

1.5. Hypothesis and Research Questions

It is hypothesized that a change in gasifier parameters like temperature and pressure will increase the yield or concentration of syngas. The validation of this hypothesis will require the answering of the following research questions:

- a) How will changing the temperature of the reactor affect the syngas yield and purity?
- b) To what extent will an increase in pressure concentration impact the rate of syngas production?
- c) How would changing the equivalence ratio impact the yield of syngas?
- d) What would be the effect of oxygen percentage on the syngas purity?

1.6. Scope of the Research

The methodology for this research involves improving the yield of syngas by simulation and modelling and testing the results in a lab scale plant. This study will consider the following;

The methodology for this research will involve performing sensitivity analysis using the Aspen plus® software. Secondly, perform process integration so that the environmental performance and efficiency of the process are improved. Data will be collected through the linkage of MS Excel TM with, Aspen plus®. In this manner, the required parameters for the calculation of performance indicators from Aspen will be directly accessible (Emun *et al.*, 2010).

Economic (efficiency) or environmental (emissions) are the performance indicators that will be used. Emission levels of SO₂, CO₂, and NO_x per unit of net

power output will constitute the environmental indicators. The gasification performance will be measured by carbon conversion and cold gas efficiencies. Nonetheless, the efficiency of the overall process will be indicated by thermal efficiency (Emun *et al.*, 2010).

1.7. Significance of the research project

In 2003 in the U.S. only, Waste-to-Energy (WtE) technologies generated 440 trillion BTU of consumable energy from MSW. This amount represented approximately 0.4% of the overall U.S. energy demand (Kwon *et al.*, 2009). Even though gasification is not as widespread and well known as the combustion technique within the WtE industry, it is still a promising alternative method.

The importance of focusing on optimizing syngas production from waste plastics is to improve analysis of the quality of the syngas produced from an IR reactor and the applicability of the developed system. Furthermore, it is to ameliorate the transformation of waste plastics into syngas as well as the heating value of the gas produced for electricity generation. Consequently, it will improve the efficiency of gasification of waste plastics as well as reducing environmental pollution caused by waste plastics. As a result, the current work will attempt to propose an alternative way to supplement energy production.

1.8. Thesis Outline

This work is constituted of seven chapters and an appendix section. The seven chapters are arranged in the following manner:

- **Chapter 1:** This introduces this work and gives a background to the project. It raises awareness of the problem investigated and elucidates the objectives of the study, the problem statement, the significance of the research project.
- **Chapter 2:** This reviewed previous literature on this work. A collection of theoretical information about thermal processes applied to waste plastic was established. Major attention was given to the gasification process since it constitutes the technology that would be used in this work. Then

attention was given to synthetic gas (syngas) and applications since it is the product of interest in this research work.

- **Chapter 3:** This describes the model of a small laboratory-scale gasification plant and also introduces the system design. It does this by presenting the various experimental equipment, mathematical development, and energy balance.
- **Chapter 4:** This addresses the modeling and simulation process. It first presents an overview of process modeling, then develops an approach for this work, and finally performs simulation analysis. The tool used in this work to perform the simulation is the Aspen plus® Software Package Version10.
- **Chapter 5:** This deals with the experimental system and material characterization. Primarily it provides an experimental procedure on how the experiment was conducted, then it also provides a characterization of the feedstock used in this work. This characterization is constituted of various analyses such as the Differential Scanning calorific, the Thermogravimetric, and Fourier transform infrared analysis.
- **Chapter 6:** This is devoted to demonstrate and discuss the findings of this work. Various results are provided based on the parameters studied.
- **Chapter 7:** This presents a conclusion from this work, made some recommendations, and suggested some further studies that could emanate from this work.

2. Chapter 2: Literature Review

2.1. Introduction

This chapter provides a review of syngas and gasification processes. Massive urbanization and rapid economic growth have led to a dramatically increasing MSW generation. Consequently, the quest for economically feasible and environmentally benign methods to minimize MSW disposal has become an urgent challenge globally (Niu et al., 2013). In this regard, gasification technology is seen as one of the promising candidates which will not only remediate the MSW disposal problem but increase syngas production as well (Kwon et al., 2009).

2.2. Plastics

Plastics invention is a ground-breaking revolution that positively impacted human life. It was first synthesized in the early 1900s and since then has replaced several types of materials including, metals, ceramics, and wood in the production of consumer products. Plastics have a variety of applications; they are easy to process and have a low cost. Furthermore, plastics are durable, light, and resistant to corrosion. Apart from their numerous benefits, researches revealed that plastic based-products are the cause of the reduction in the cost of production in many industrial sectors (Hoornweg & Bhada-Tata, 2012). This argument is supported by Pinto et al., (1999) who stated that the enormous production of plastics is based on the fact that plastics are needed in electronics, automobiles, households, agriculture, toys, packing materials, and several other applications. As indicated by Plastic Europe, the world's production of plastic in 2011 was above 280million tons and yet it was still exponentially increasing. This is mainly due to the fact that plastics have a large range of applications, have incomparable usability, have non-degradable nature, and a low cost (Sriningsi et al., 2014).

Plastics are petroleum derivatives. In other words, plastics can be defined as a long hydrocarbon chain of an organic compound synthesized from petroleum products. And even though plastics have tremendous advantages and have considerably improved the quality of human life; they remain a severe threat to the continuation of life on earth. This argument is corroborated by Subramanian (2000) which revealed that plastic is more harmful than beneficial to the

environment. Hidayah, (2018); Raja & Murali, (2011) showed that the increasing demands of plastics have instigated an accumulation of plastic wastes in landfills, consequently consuming a lot of space and generating environmental pollution. Subramanian (2000) highlighted certain causes of increasing human dependency on plastics, including development and economic growth.

2.2.1. Waste Plastics

In the last three decades, plastics generation has expanded worldwide due to their numerous applications in different sectors. This expansion has caused an accumulation of waste plastics in landfills (Sharuddin., 2018). Consequently, causing a high risk on human and animal health, as well as imposing severe damage to the environment by generating greenhouse gases and polluting groundwater. In this regard, one of the greatest challenges that developed and developing countries are currently faced with is the disposal and management of their waste plastics.

A survey conducted in 2012 by the India Central Pollution Control Board reported that approximately 5.6 million tons of waste plastics were generated each year in India. Of that amount, nearly 60% is reused or recycled. The remaining 6500 tons of waste plastic is disposed of in landfills daily. Since there are several plastic-based materials accessible on the market and consequently on the waste stream, plastics are grouped into two major categories namely thermosetting (long strands) and thermoplastic (short link) (Sharuddin et al., 2018). Thermoplastic is the group of plastics that can be recycled whereas thermosetting is that one cannot be recycled subsequently generating an enormous waste of plastic and in the current context of climate change, environmental pollution awareness, it is safe to arguably mention that waste plastic treatment has become unavoidable and imminent. Generally, waste plastics can be divided into at least two main categories namely municipal and industrial waste plastics.

Municipal waste plastics have various sources such as domestic items (e.g. CDs and cassette boxes, food containers, disposable cups packaging foam, drainage pipe, plates, wire and cable, carbonated drinks bottles, cutlery, fridge liners, electronic equipment, flooring, cushioning foams, vending cups, thermal insulation foams, plumbing pipes and guttering, surface coatings, etc.). In addition to that, there is agriculture that is also an enormous source for municipal plastics

waste with items such as fertilizer bags, mulch films, feed bags, covers for hay, silage, etc.). Another huge source of municipal plastic wastes generation is automobile wrecking (Passamonti, & Sedran; 2012). According to Hidayah, (2018), the majority of municipal waste plastics come from household waste, hence, in order to reprocess municipal waste plastics, certain classification processes must first be undertaken. For instance, a wet-based separation process could take place first. This means mixed plastics can be arranged in two groups. Namely the plastics with a density above that of water and the plastic with a density lesser than the one of water. Examples of plastics with a density bigger than the one of water are polyvinyl chloride and polystyrene. As for plastics such as expanded polystyrene, polyethylene, and polypropylene, they have a density lower than that of water. Hence, when the treatments of waste plastic deal with mixtures such as polystyrene, polypropylene, and polyethylene, it shows that the above classification processes are experienced. Even though several studies and researches have been undertaken on MSW separations technologies, the challenge of finding marketable portions and categorize MSW mechanically still remains high. Consequently, household waste categorization is critical. Solid household waste is categorized into (i) incombustible such as metals, ceramics, glass, (ii) combustibles namely textiles, wood, paper, and kitchen waste, and finally (iii) plastics (Demirbas., 2004).

Industrial Plastic Wastes is mostly called primary waste. It is the group of plastics that originate from large industries such as the plastics processing industry, the manufacturing industry, and the packaging industry. The companies generating the most industrial plastic wastes are the demolition and construction companies that produce waste plastic constituted of plastic pipes and fittings as well as sheets and tiles. Another big sector that releases an enormous amount of plastic waste is electronics and electrical companies. They produce plastic waste such as TV screens, cassette boxes, cable sheaths, switch boxes, etc. One sector that cannot be neglected in its waste plastic production is the automotive sector. Indeed, automotive companies produce elements like car spare parts, battery containers, front grills, and several others. One advantage that needs to be highlighted about primary waste or industrial plastic waste is that their physical

characteristics are relatively good. They are contaminant-free as they are clean enough in production and are available in sufficient quantities. Industrial plastics are more homogenous and free from contamination whereas municipal plastics are more heterogeneous and are not contamination-free. Due to their homogenous and free contamination characteristics, industrial plastics are recycled into low-grade plastics products (Zhou et al., 2014) while municipal plastic wastes with their heterogeneous and the fact that they are contaminated or also consist of mixed resins are not suitable for reclamation. In this regard, one of the best methods for recycling those would be through thermal cracking into hydrocarbons (Demirbas, 2004).

According to Lettieri & Al-Salem (2011), plastics are approximately 10.6 ±5.1wt% of municipal wastes. Low-density polyethylene (LDPE), high-density polyethylene (HDPE), polypropylene (PP) polyvinyl chloride (PVC), polyethylene terephthalate (PET), and polystyrene are the primary constituents of municipal plastics waste (Zhou et al., 2014). In general, packaging material derivatives of polystyrene, polyethylene, polyvinylchloride, and polypropylene constitute nearly 50-70% of the global plastic waste (Scott et al., 1990). Polyethylene constitutes the largest fraction (69%) of all plastic wastes and 63% of the total packaging waste (Lettieri & Al-Salem, 2011; Scott et al., 1990).

Recent studies and scientific research have particularly been interested in new ways of environmentally-friendly methods for treating waste plastics. Among those technologies, the use of the gasification process for the recycling of waste plastics has been of major interest. The following sections focus on gasification technology, its advantages, and its disadvantages.

2.3. Gasification process basis features

The gasification process can be viewed as a process where thermochemical conversion processes involving various chemical reactions under conditions of high pressure, heat, and mass transfers (Widjaya et al., 2018). Gasification technology is a process that has been used since the 19th century. It was used in Europe in the early 1900s for fuelling cars during fuel shortages. Currently, gasification is intensively used as an alternative technology for waste management.

2.3.1. Process types

According to Arena & Mastellone (2009); E4tech (2009); Higman & Van der Burgt (2003), gasification is known as a multifaceted process that contains several chemical and physical exchanges that take place at temperatures usually greater than 600°C. They further stated that the gasification exact temperature depends on the waste characteristics, more especially the melting temperature and the ash softening. It also mostly depends on the reactor type. The gas obtained from gasification is known as syngas and mostly contains hydrogen (H₂), carbon monoxide (CO), methane (CH₄), and a significant amount of inert gas such as carbon dioxide (CO₂) (Widjaya, et al., 2018).

Classification of gasification processes is usually based on the type of oxidation medium. In this regard, there are numerous oxidation mediums among which are, partial oxidation with air, pure oxygen or oxygen-enriched air, plasma gasification, and steam gasification. When partial oxidation with air is used as an oxidation medium, it generates a producer gas contaminated with atmospheric nitrogen up to about 60% and a calorific value between 4 and 7 MJ/m³N. According to Arena (2012), for a gas turbine to operate, it required gas with a calorific value approaching 38 MJ/m³N. Unfortunately, partial oxidation with air could not provide such high values subsequently, it was considered too low to be utilized. Nevertheless, it is currently possible to easily find gas turbines that if partially cooled and adequately cleaned, can efficiently burn syngas with low heating value (Arena, 2012). According to Mastellone et al., (2010), in order to achieve a higher heating value, certain processes were run with oxygen-enriched air. Those processes were run with a mixture of oxygen (20-50%) and nitrogen. The fact that there is less nitrogen content results in creating an auto-thermal process at greater temperatures without wasting oxygen.

In partial oxidation with pure oxygen, syngas free from atmospheric nitrogen with a higher calorific value between 10 and 15 MJ/m³N, is generated. This renders additional investment and operating costs for oxygen production unnecessary and unjustified unless the production capacity is meant to be above the 100 kilotons per year. The obtained higher heating value syngas is characterized by reduced low tar content, volumetric flow rate, and, in particular,

vitreous ash production that is responsible for nuisance in disposals. On the other hand, the steam gasification process generates high hydrogen concentration (40%) (Szwaja, et al; 2019). It also generates a medium heating value (15–20 MJ/N m³), as well as nitrogen-free syngas. The only gasifying agent present in the steam gasification process is steam. Additionally, the process has no exothermic reactions taking place subsequently, it requires an external source of energy for endothermic reactions to occur (Arena, 2012).

In plasma gasification, the heating source is one or more plasma arc torches that generate an electric arc and yield high-temperature (15,000°C) plasma gas (Moustakas et al., 2005; Lemmens et al., 2007). This, in turn, allows for control of temperature to be independent of variations in the feed supply and quality of a gasification agent such as air, oxygen, or steam. Consequently, varying elemental composition, moisture content, and feeding rate are allowed in the waste materials. Different particle sizes including fine powders and coarse lumps can be accepted as feedstocks of plasma gasifiers with minimal feed preparation (Gomez et al., 2009).

2.3.2. Process steps

Arena (2012), describes solid waste gasification as a sequence of successive exothermic and endothermic steps. These steps are schematically illustrated in figure 2-1 (Knoef, 2005; De Souza-Santos 2010). The exothermic reactions are taking place during the combustion steps and the endothermic reaction are taking place during the gasification and pyrolysis steps. As further illustrated in figure 2-1, the heat generated during the exothermic step (combustion) is used as a reactant during the endothermic steps (gasification and pyrolysis).

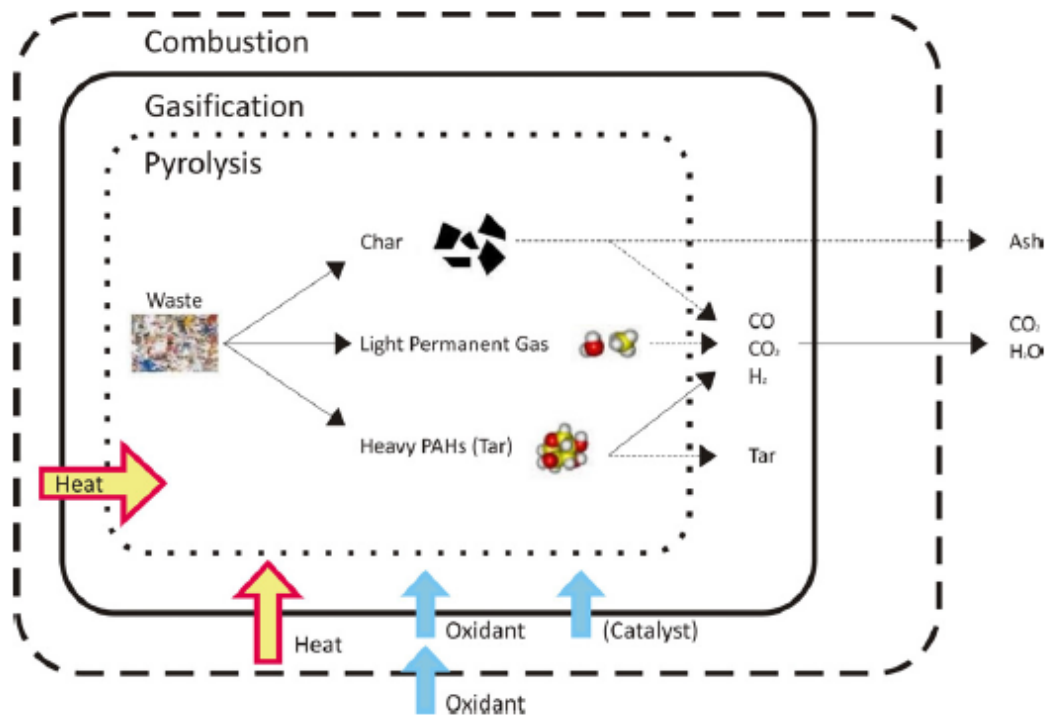


Figure 2-1: Schematic Representation of Gasification, pyrolysis, and combustion steps (Arena, 2012)

Even though there is a multitude of gasification reactions, it is possible to distinguish three autonomous gasification reactions (Table 2-1): The Boudouard reaction (reaction 1), hydrogasification (reaction 14), and water-gas reaction (reaction 10).

Table 2-1: Solid Waste Gasification process main reaction during homogenous and heterogeneous phase (Arena U 2012)

Carbon reaction involving carbon dioxide		Mj/Kmol	
1	$\text{CO}_2 + \text{C} \rightleftharpoons 2 \text{CO}$	+172	Boudouard reactions
2	$n\text{C} + \text{C}_n\text{H}_m \longrightarrow m/2 \text{H}_2 + 2n\text{CO}$	Endothermic	Drying reforming
Oxidation reactions			
3	$\text{C} + \text{O}_2 \longrightarrow \text{CO}_2$	-394	Carbon oxidation
4	$\text{C} + \frac{1}{2} \text{O}_2 \longrightarrow \text{CO}_2$	-111	Carbon partial oxidation
5	$\text{C}_n\text{H}_m + n/2 \text{O}_2 \longrightarrow n\text{CO} + m/2 \text{H}_2$	Endothermic	C_nH_m Partial oxidation
6	$\text{CO} + \frac{1}{2} \text{O}_2 \longrightarrow \text{CO}_2$	-283	Carbon monoxide oxidation
7	$\text{H}_2 + \frac{1}{2} \text{O}_2 \longrightarrow \text{H}_2\text{O}$	-242	Hydrogen Partial oxidation

Gasification reactions involving steam

8	$C_nH_m + nH_2O$	\longrightarrow	$nCO + (n + m/2)H_2$	Endothermic	
9	$CO + H_2O$	\longrightarrow	$H_2 + CO$	-41	Water-gas shift reaction
10	$C + H_2O$	\longrightarrow	$H_2 + CO$	+131	Water-gas reaction
11	$CH_4 + H_2O$	\longrightarrow	$3H_2 + CO$	+206	Steam methane reforming

Decomposition reactions of tars and hydrocarbons*

12	pC_xH_y	\longrightarrow	$qC_nH_m + tH_2$	Endothermic	
13	C_nH_m	\longrightarrow	$nC + n/2 H_2$	Endothermic	

Gasification reactions involving Hydrogen

14	$2H_2 + C$	\longrightarrow	$2CH_4$	-75	Hydrogasification
15	$3H_2 + CO$	\longrightarrow	$H_2O + CH_4$	-227	Methanation

* Note that C_xH_y represents tars and, in general, the heavier fuel fragments produced by thermal cracking, and C_nH_m represent hydrocarbons with a smaller number of carbon atoms and/or a larger degree of unsaturation than C_xH_y .

2.3.3. Gasification parameters

Several parameters affect the gasification process. Namely the pressure, the reactor size particularly the reactor bed height. There is also the temperature, the equivalence ratio, the fuel's characteristics, the fluidization velocity, and the air-to-steam ratio. All these aforementioned factors when interacted affect the outcome of the gasification products. For instance, Sadaka (2017) reported an increase in the production of combustible gases after increasing the temperature. He further added that an increase in temperature plays an important role in the energy content of syngas as it also increases. As for the pressure, it plays a role in the gasification char. As the pressure increase, so is the rate of gasification char. The reactor size plays an impact based on the reactor bed. Indeed, a higher fuel bed means better residence time and consequently an increase of the total syngas yields and increases in the concentrations of carbon dioxide, hydrogen, carbon monoxide, and methane.

2.4. Gasifier

Gasification processes take place in a gasifier. Flow arrangement of the fuel source and produced gases are certain characteristics used to classify gasifiers

(Widjaya et al. 2018). There is a huge variety of gasifiers available on the market. The selection of the gasifier type is an extremely important parameter in the success of the gasification process. Fixed bed, entrained flow bed, and fluidized bed are the most frequently used type of reactor vessel for gasification processes (Li, G et al., 2018). The following sections detail these three vessels.

a) Fixed-Bed Gasifier

A fixed bed type gasifier is also known as a moving bed gasifier. It is the simplest type of gasifier (Widjaya et al., 2018) as it is determined by the natural flow of fuel through drying, pyrolysis, gasification, and combustion processes. It favors direct contact between the gases and the fuel particles. Furthermore, fixed bed gasifiers are primarily characterized by the requirement of low oxidant concentration and also by generating high methane concentration in syngas, and finally releasing liquids like tar and oils. The product of the fixed bed is syngas containing a little amount of tar and having high temperature and medium caloric value. The main demerit of fixed bed gasifiers is that they cannot handle high moisture content and wide particle size distribution (Mbourou, 2016). Figure2-2 presents two fixed bed gasifiers. The first one (left) is a counter-current fixed bed gasifier, meaning the feedstock and the gasification medium flow in a counter-current manner. The second fixed bed gasifier (right) is a co-current one. It feedstock and gasification medium flow in the same direction.

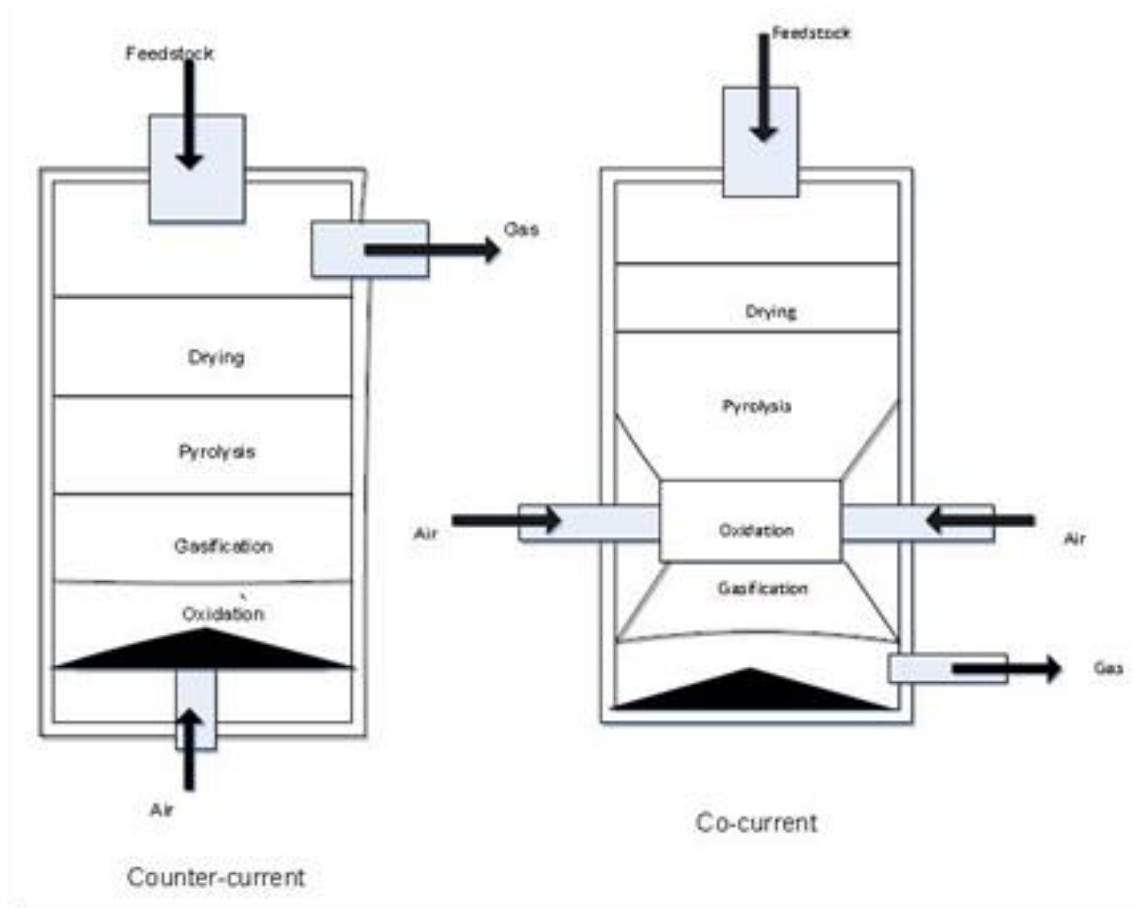


Figure 2-2: Illustration of fixed bed gasifier (Mbourou, 2016)

b) Fluidized-Bed Gasifier

A fluidized bed gasifier is characterized by a constant mixing process happening between the old and new particles, as well as between partially and fully gasified particles (Mbourou, 2016; ómez-Barea & Leckner., 2010; Belgiorno et al., 2003). This process of constant mixing is extremely advantageous as it results in an increase in the residence time of particles and consequently an increase in the production efficiency of the fluidized bed. This great mixing or recycling characteristic added to the reaction rate and the possibility to be built in bigger size rendered fluidized bed gasifier way advantageous than fixed-bed gasifiers (Gómez-Barea, & Leckner., 2010).

Figures 2-3 showcase two types of fluidized bed gasifiers. The first one (a) is a bubbling type of fluidized bed gasifier also known as BFBG and (b) is a circulating type of fluidized bed gasifier also known as CFBG. The difference between these two types resides in the velocity. While CFBG operates at a velocity

ranging between 2-5m/s, BFBG whereas operates at a velocity ranging between 0.5-2m/s (Gómez-Barea, & Leckner., 2010).

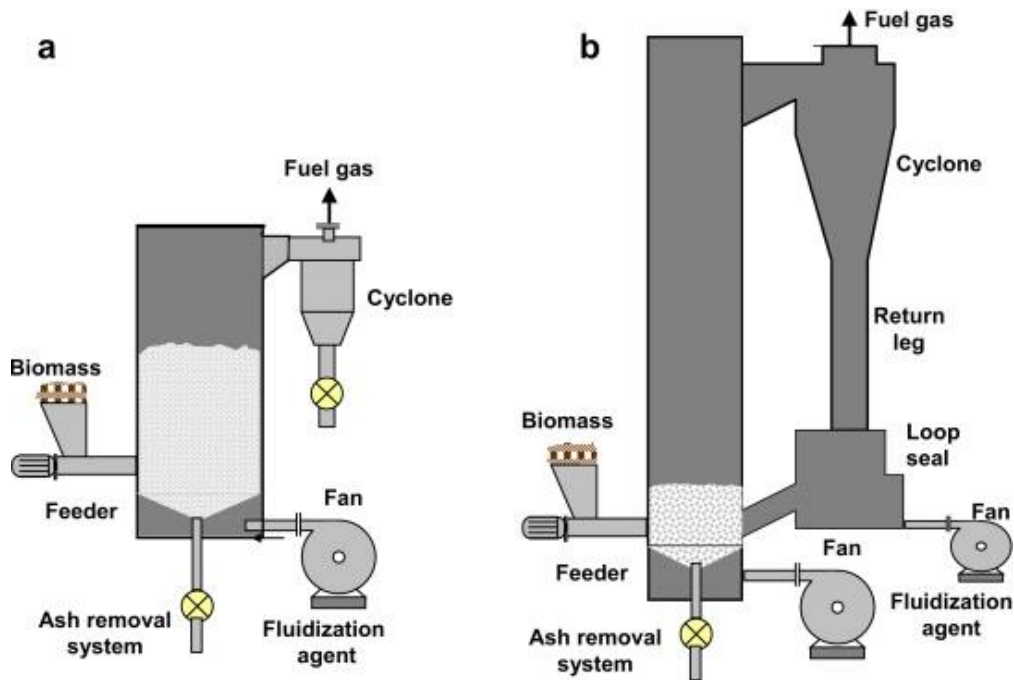


Figure 2-3: Illustration of two fluidized bed gasifiers (a) Bubbling (b) Circulating (Gomez-Barea & Leckner, 2010)

c) Entrained-Flow Gasifier

The Entrained-flow gasifier has a residence time that ranges in the order of seconds. As represented in figure 2-4, the feedstock is injected with oxygen or air and they rapidly react as they moved down the gasifier. This very short residence time forces the entrained-flow gasifier to operate under high temperature (1200-2000°C) thus, achieving its high carbon conversion level. In comparison to the fluidized-bed and fixed-bed gasifier, this gasifier has the shortest residence time and consequently the lesser fuel particle contact (Widjaya et al.,2018; Mbourou, 2016).

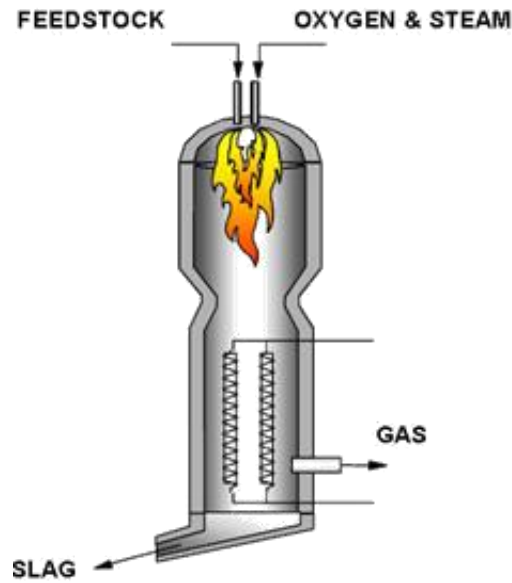


Figure 2-4: entrained-bed gasifier (Kurkela, 2010)

2.5. Comparison between gasifier types

There are various types of gasifiers available and each one has its advantages and disadvantages. Tables 2-2 present a brief comparison among certain gasifiers. It highlights each gasifier's benefits and introduces each one drawback.

Table 2-2: Comparison between gasifiers (adapted from widjaya et al., 2018 and Brain 2003)

Gasifier	Advantages	Disadvantages
Fluidized bed	Large scale applications	Medium tar yield
	Feed characteristic	Higher particle loading
	Direct/indirect heating	Excellent mixing characteristics
Fixed-bed (downdraft)	Can produce syngas	Feed size limits
	Small scale applications	
Fixed-bed (updraft)	Low particulates	Scale limitations
	Low tar	Producer gas
	Mature for heat	Moisture sensitive
		Feed size limits
	High Moisture can be handled with Small scale applications	High tar yields
	Ash does not contain carbon	Scale limitations
		Producer gas
Entrained-flow	Possibility of scaling for low tar. Syngas Can be produced	Slagging potential
		A large amount of carrier gas
		The loading capacity of the particle is higher

2.6. The Benefits of the Gasification Process

Benefits of the gasification process highlighted in the literature (Rusell, 2001; Arena & Mastellone, 2006; Arena, 2012; Stiegel & Belgiorno et al., 2003; Brems et al., 2013) are summarized below:

- Gasification has the potential of producing low-cost electricity sources using solid wastes as feedstock. This renders it an environmentally friendly technology.
- There is flexibility in both products and feedstock with gasification. Further to that, the flexibility of the gasification process allows for a wide range of feedstock to be used in the reactor for waste plastic gasification.
- The capacity to generate fewer solid waste.
- Rather than relying on oxygen, gasification relies on air.
- The gasification reactor allows for high pressure and temperature.
- The by-products of the gasification process are harmless solid remains, that can be used as building construction materials. Hence, they do not constitute another source of disposal cost, or better if their processing is further advanced, they produce value-added elements.
- With gasification technology, polymers like plastics are entirely broken down into simple components such as syngas.
- Products resulting from gasification without adding further disposal costs can be automatically disposed of into landfills as they are harmless.

2.7. Drawbacks of gasification

The gasification process does not only have advantages. It also has disadvantages which are listed below (Wu & Williams, 2010; Arena, 2012; McKendry, 2002; Consonni & Viganò, 2012):

- Separation processes need to first take place due to the diversity of waste items.
- The reactor dictates the limits of the feed size.

- The sulfur content from the gas released out the gasification process could be high.
- The gasification process is very moisture sensitive.
- The need for further treatment of syngas.

2.8. Syngas

Syngas is a combustible gas mixture containing various gases (Consonni and Viganò, 2012). Syngas compositions depend on several parameters such as the feedstock, the reactor temperature, and numerous others. He et al., (2009) reported that for syngas production from catalytic gasification of waste polyethylene, the concentrations of syngas components were hydrogen (H₂) 16.92-36.98%, carbon monoxide (CO) 20.33-27.37%, carbon dioxide (CO₂) 35.28-20.78%, and methane (CH₄) 21.44-9.94%. The presence of various gases in syngas makes it a good feedstock in a wide range of applications. Figure 2.5 here below presents some of these applications. The various gases that constitute the syngas mixture are N₂, H₂, CO₂, CH₄ and CO. One important application of syngas is the generation of electricity. Due to the composition of methane and hydrogen, syngas can be used as a fuel system to generate steam or electricity.

A study conducted by Luo et al., (2012) on syngas production through catalytic steam gasification of MSW in a fixed-bed reactor and focusing on the influence of steam to carbon ratio (S/C), the effect of the catalyst, and the reactor temperature on the gas yield, reveals that temperature significantly affects the catalytic steam gasification. This means while the reactor temperature increases, the production of syngas increases including the carbon conversion efficiency as well. The study further revealed that it is at 900 °C that the highest gas yield was obtained. Three factors could fundamentally explain the increase of the gas yield with temperature. (i) As the temperature increased, the initial pyrolysis is faster and the syngas production is greater. (ii) The rate at which endothermic reactions of gasification of char are taking place and finally (iii) An increase in reforming and steam cracking of the tars.

In order to be able to identify the conditions at which wood gasification syngas is optimized and determine their syngas composition Begum et al., (2014),

performed pilot-scale gasifier experiments. Their study consisted of using software and investigate the influence of steam fuel and air ratio on gas composition. They did that by developing and validating a numerical model. The performance variation between their experimental results and their simulation was a maximum of 3%. Patterning the results, they demonstrated that an increase in air quantity creates a decrease in hydrogen and carbon monoxide gases. But also generate an increase in the volume of nitrogen contained in the syngas. The results further demonstrated that while CO₂ concentration reduced with minor deviation, the CH₄ amount remained nearly unchanged. The oxygen amount fed in the reactor, and the gasification temperature, are represented by the air-fuel ratio. An increase in oxidation reaction with a high air-fuel ratio can lead to the degradation of the quality of syngas. There is a directly proportional relationship between gasification temperature and fuel ratios and consequent acceleration of the gasification process and better product quality.

2.9. Syngas Application

Syngas has numerous applications from chemicals to energy generation. The figure below best summarizes the various and diverse applications of syngas. This rich and multifaceted syngas application makes it a very valuable resource. For instance, as indicated in Figures 2-5, syngas can be used as raw material for the production of methanol which itself is a raw material to many other chemical products such as ethylene, acetic acid, formaldehyde, and many others. Syngas can also be used for power generation through the Integrated Gasification Combined Cycle (IGCC) or the steam and power. Another application syngas can be used for are hydrogen generation for the production of ammonia, chemicals, and fuel cells. Syngas is also useful through the Fischer-Tropsch process to produce naphtha, petrol, diesel, and wax. There are numerous methods and technologies available to produce electricity from synthetic gas, namely combustion engines, and gas turbines. One particular advantage of using gas turbines for the production of electricity is their capacity on having high efficiency and low capital cost. This is even more accurate when operating on a small-scale application (Bridgwater et al., 2002).

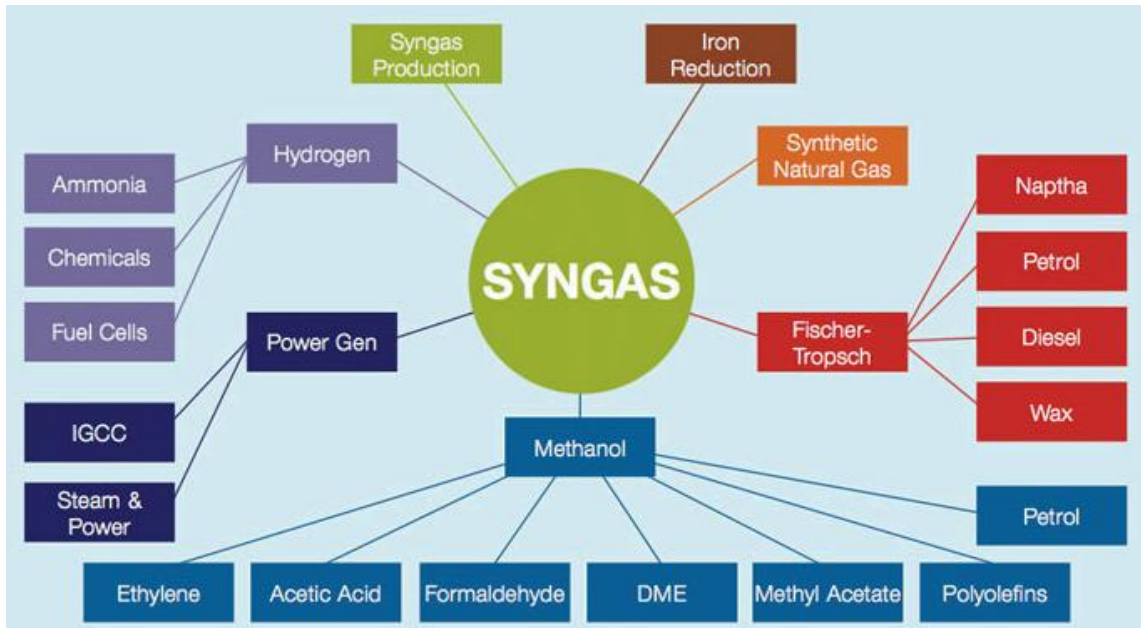


Figure 2-5: Illustration of Synthetic Gas Application (WtE, 2020)

3. Chapter 3: Gasification Plant and System Design

3.1. Description of the gasification Plant

The gasification plant is a small laboratory scale plant. It aims to generate power. The gasification plant is constituted of an IR reactor which is responsible for the gasification of the feedstock, and a catalytic water gas shift (WGS) system which is responsible for enhancing hydrogen production via the concentration of syngas thermal energy. The waste plastic feedstock is pelletized and separated according to their density, low-density polyvinyl ethylene (LDPE) or high-density polyvinyl ethylene (HDPE).

The plant design (Figure 3-1) is based on a process that is capable of producing fuel from waste plastic materials using an infrared reactor composed of ceramic heaters to gasify the waste in order to generate syngas. The synthetic gas produced could then be further processed and converted into pure hydrogen which would be stored in a fuel cell.

3.2 System Design

3.2.1. Experimental Equipment

a. Reactor Description

The gasifier used for this project is a packed bed infrared reactor (IR reactor), equipped with four 125×125 mm electric infrared ceramic heaters (model UHI-LYTHTS-0250, ELSTEIN, Johannesburg, South Africa). The reactor is composed of three sections. A cone on top, a tube with a hole, and the four heaters are connected in the middle around its wall (Figures 3.2). The reactor mesh is attached to a disk at the bottom section. The total height of the reactor is 680mm, including a tube length of 336 mm and cone height of 344 mm. The internal and external diameters are 300 mm and 330 mm in that order. The reactor in its entirety is made out of stainless steel material. A fiber blanket is used as heat insulation and placed between the tubes. This fiber blanket can withstand a temperature of 1300 °C. A removable holding tray is placed at the bottom of the tube to hold the plastic pellets (feedstock). It is made of a fine wire mesh and has the shape of a cylinder with 250mm height and 200mm diameter. All four heaters are set to a temperature of 700 °C. The reactor is assumed to be airtight and the gasification process occurs at standard atmospheric pressure.

The various schematics below represent the different views of the gasifier design. Figure 3.2a represents a front-cut view of the design, whereas figure 3.2b represents the external view. Figure 3.2c represents the inner view of the reactor from the bottom. Figure 3.3 is the visual view of ceramic heaters mounted on the reactor wall. Table 3.1 gives a description of the reactor dimensions.

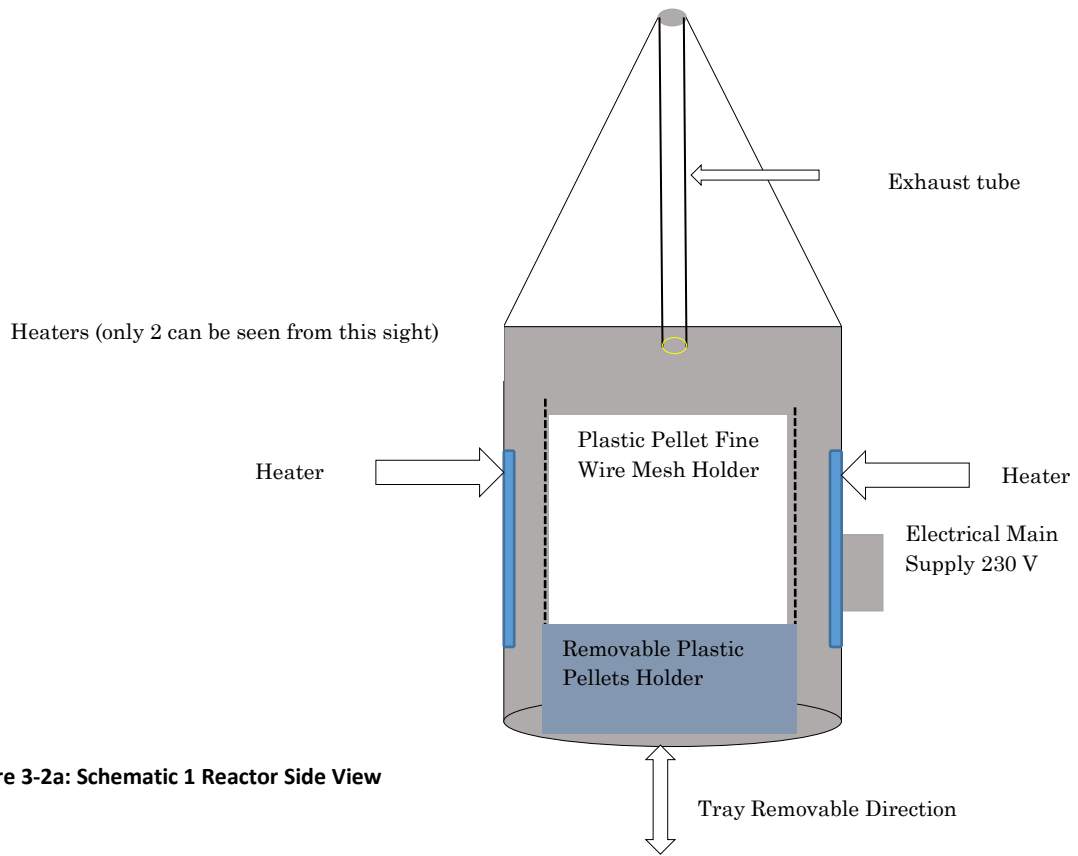


Figure 3-2a: Schematic 1 Reactor Side View

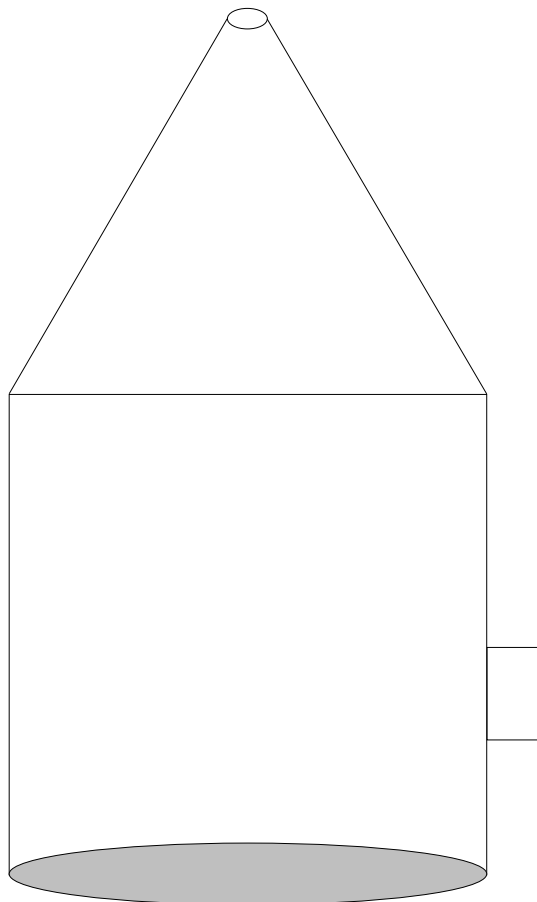


Figure 3-2b: Reactor external view

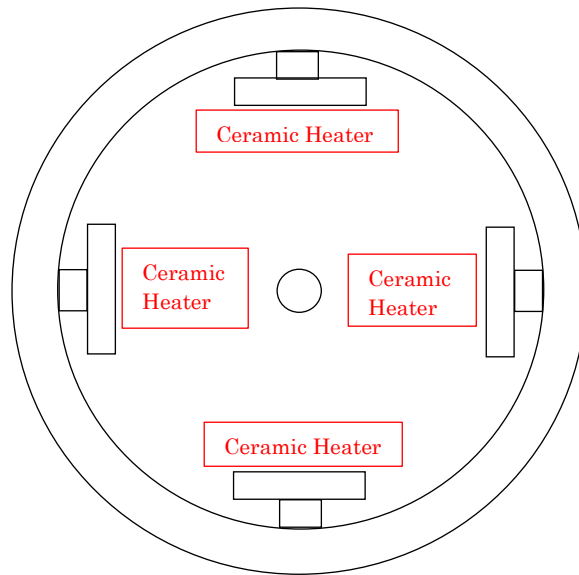


Figure 3-2c: Internal view from the Bottom



Figure 3-3: Physical view of the reactor and the heaters

Table 3-1: Reactor Description

Description	Size (mm)
Heater	125×125
Material thickness	30
Mesh bucket diameter	178
Mesh bucket length	270
Reactor exhaust diameter	25.4
Reactor Height	680
Reactor Length	330
Smoke Hole diameter	20

b. Electric Infrared ceramic heaters

The design of electric IR ceramic heaters depends on their shape and the effectiveness of reflectors. They are also designed with a coiled heating element wire such as aluminum, chrome, or iron alloy which have high emissivity. The objective of electric IR ceramic is to pass electric current across the filament. An important portion of the input power emerges through convection as heat. The efficiency and characteristics of the ceramic heater are determined by the filament. Usually, operating on a scale ranging between 300°C and 700°C, IR ceramic heaters have wire embedded inside the ceramic materials. This prevents any attack by atmospheric oxygen and also protects against thermal shock. The conception of the entire system is made so that damages, oxidation, and corrosion are prevented (Das & Das, 2010). The wave spectrum of IR heaters varies from medium to long waves. They have an efficiency of approximately 95 %. Das & Das (2010) indicated that 3.3-5.7 μm is the peak range of radiation.

c. Plastic Pellets

Mastellone & Zaccariello (2015) reported several unique aspects related to the thermal treatment of plastic waste. These include:

- The stickiness of the molten polymer
- The very low content of ashes
- The low specific heat volume of the solid polymer
- The very low content of char

Following the plastic pellets feed into the reactor, is a very fast heat transfer mechanism leading to the external surface of the pellet to soften. The time necessary to reach the softening stage can be determined using the dynamic energy balance method on a single plastic pellet as given in equation (3-1). The properties of polyethylene and parameters of thermo-optical used for energy balance are presented in Tables 3.2 and 3.3.

$$m_{fuel} \cdot C_p \cdot \frac{dT}{dt} = A \cdot h_{bed} \cdot (T_{bed} - T_{melting}) - r_{melting} \Delta H_{melting} \quad (3-1)$$

where

C_p = specific heat of the fuel

$\frac{dT}{dt}$ = Temperature of the pellet surface (depends on time)

A = external Area of the Pellet

h_{bed} = heat transfer coefficient between bed and pellet

T_{bed} = bed Temperature

m_{fuel} = mass of the fuel

$T_{melting}$ = Temperature at which the plastic melt

$r_{melting}$ = rate of melting

$\Delta H_{melting}$ = the latent heat of melting

The general solution of energy balance as expressed by Mastellone & Zaccariello (2015) is given here below in the equation (3.2) and (3-3):

$$T(r) = T_{bed} + (T^o - T_{bed}) \cdot \exp\left(-\frac{h_{bed} \cdot A}{m \cdot C_p}\right) \quad (3-2)$$

$$h_{bed} = \frac{N_u \cdot K_{fuel}}{d_{fuel}} \quad (3-3)$$

Where

N_u = Nusselt number

K_{fuel} = fuel conductivity

d_{fuel} = fuel pellet diameter

The equation for convection by the surrounding gas produced in the IR reactor is given by:

$$H_{conv} = \alpha \cdot A \cdot (T - T_g) \quad (3-4)$$

Where

T = Temperature of the plastic in kelvin

T_g = Temperature of the outlet gas in kelvin

α = Heat transfer coefficient (convective)

A = Area of the surface in m^2

Table 3-2: Thermo-optical Parameters

Properties	LDPE	HDPE
H (J/kg)	0.572	0.801
ρ (g/cm³)	0.92	0.96
C_p (J/kgk)	3180	3640
K (W/mk)	0.34	0.49

Table 3-3: Properties of Polyethylene needed for energy balance. Adapted from (Mbourou, 2016)

Parameters	Values	Units
Fuel Conductivity (k_{fuel})	0.46	cal/s m °C
Fuel Density (ρ_{fuel})	950	kg/m ³
Fuel diameter (d_{fuel})	0.005	m
Conductivity of Gas (k)	0.016	cal/s m °C
Density of Gas (ρ)	0.315	kg/m ³
Viscosity of Gas (μ)	4.91E-05	Ns/m ²
Fuel's Melting heat ($\Delta H_{melting}$)	23.8	kcal/kg
Fuel Softening temperature	135	°C
Fuel Specific heat (C_p)	0.55	kcal/°C kg
Temperature (T)	Would be obtained during simulation	°C

3.3. Mathematical Development of IR Reactor.

From the food industry to commercial building and household needs, heaters have several applications. The design and commercialization of heaters depend upon their application. Hence, the filament resistivity and temperature increment are proportional. This leads to reduction in current and power consumed by the heater (Roth & Brodrick, 2007).

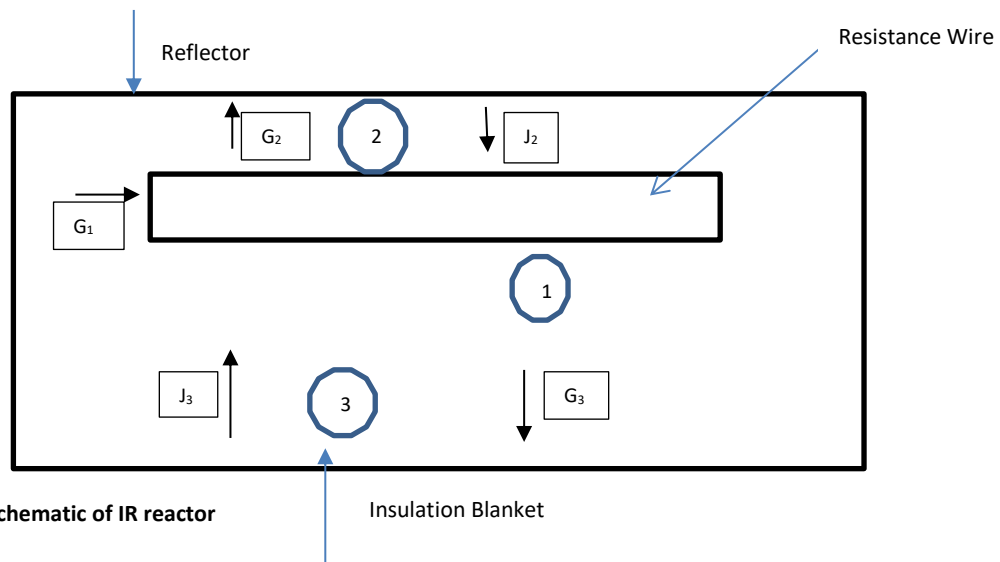


Figure 3-4: Schematic of IR reactor

According to Mbourou & Adonis (2012), the heat transfer radiation in this type of heater is similar to the one suggested by (Pettersson & Stenstrom, 2000). In their study, Pettersson & Stenstrom (2000) assumed for simplification purposes that the exchange model will have to be non-grey and radiation is to be diffused.

The rise in temperature in the resistive filament is a product of heat transfer by conduction that is taking place around the surroundings. Its equation is expressed as follow:

$$i(t) = \frac{U}{R}(1 - e^{k_1}) + C_2 e^{k_2} K_{1,2} = -\frac{1}{RC} \left[1 \pm \sqrt{1 - \frac{4R^2C}{L}} \right] \quad (3-5)$$

Where C_2 is a constant and K_1 and K_2 are obtained according to the following equations:

$$K_1 = \frac{R}{L} \quad (3-6)$$

$$K_2 = -\frac{1}{RC} + \frac{R}{L} \quad (3-7)$$

From the resistive filament to the ceramic body, the heat transfer through conduction. Equation 3-8 here below would be used to calculate the heating rate of the ceramic heater.

$$T = T_1 + (T_0 + T_1) e^{2Na_r^2} \quad (3-8)$$

Where the diffusivity $a = C_p \lambda$

N = heat transfer coefficient indicating the heat exchange between the medium.

r = depth penetration of heat pulse

T = Actual temperature of the heater at $t = 60$

T_0 = Heater initial temperature

T_1 = Temperature of the medium

The heating reliability and stability of a heater are determined by its extent to remain constant over its service life.

$$\xi = \xi_0 e^{\left(\frac{-Q}{RT}\right)} \quad (3-9)$$

ξ_0 = Production constant of the material of the conducting phase

Q = Activation energy of the aging process

T = Heater operating temperature

To perform the simulations and modeling of the IR reactor the following assumptions were considered:

- The ceramic reflector and surface added to the infrared source are considered grey bodies.
- The IR reactor heat loss is negligible.
- The chamber surface where the irradiation of plastic pellets takes place is parallel with the heaters.
- No radiation is taking place, since the insulation blanket inside the IR reactor prevents heat loss.

3.4. Energy Balance

Energy balance is characterized by the transfer rate of energy from a hot surface to a cooler surface. The general expression of energy balance is defined as in Equation 3-10.

$$E_{in} - E_{out} = 0 \quad (3-10)$$

The resistance would be opposed to the thermal equilibrium of the filament wire inside the ceramic heater because of the electrical current passage. Variation in temperature of the filament wire is equal to the power lost through radiation and convection from the heater surface. The moment the current flowing through the filament becomes constant, the steady-state would be reached (i.e. the derivative of the temperature equates to zero ($dT/dt=0$)). By applying the first law of thermodynamics to a system with an electrical wire of length L, the equation would be as follows:

$$E_g - E_{out} = E_{st} \quad (3-11)$$

The above equation is comprised of E_g which corresponds to the internal energy generation originating from the electric current. It is also constituted of E_{st} , which corresponds to the change in energy storage, and finally of E_{out} which corresponds to the energy flowing out. E_g the energy generated by the electric resistant heating is expressed as follow:

$$E_g = I^2 R_e L \quad (3-12)$$

The energy generated through electric current is converted into heat and dissipates at a rate of $I^2 R$. The remaining energy caused by the net radiation while leaving the surface of the heater is given by the following equation:

$$E_{out} = \varepsilon \sigma (\pi DL) (T^4 - T_{sur}^4) \quad (3-13)$$

The energy storage caused by the change in temperature is given by equation 3-14 here below.

$$E_{st} = \frac{dU}{dt} = \rho c V \frac{dT}{dt} \quad (3-14)$$

ρ represents the density of the filament wire material

c corresponds to the specific heat of the filament wire

V is the volume of the wire and is expressed as follows

$$V = \left(\frac{\pi D^2}{4} \right) L \quad (3-15)$$

The substitution of each equation expression into equation (3-11), results in the following expression:

$$I^2 R_e L - \varepsilon \sigma (\pi D L) (T^4 - T_{sur}^4) = \rho c V \left(\frac{\pi D^2}{4} \right) L \frac{dT}{dt} \quad (3-16)$$

Hence the time rate of change of the filament wire temperature of the heater is:

$$\left(\frac{dT}{dt} \right) = \frac{I^2 R_e L - \varepsilon \sigma (\pi D L) (T^4 - T_{sur}^4)}{\rho c \left(\frac{\pi D^2}{4} \right) L} \quad (3-17)$$

The power output of the heater is given by the filament wire according to the expression:

$$P = IV = \frac{V^2}{R} \quad (3-18)$$

Where is equal to:

$$R = \rho \left(\frac{l}{A} \right) (\Omega) \quad (3-19)$$

R corresponds to the resistance

l corresponds to the length A corresponds to the Area

ρ corresponds to the resistivity and V the voltage equals 220V for a single phase.

The expression of the overall heat transfer rate is given as follow:

$$Q = \frac{P_{tot}}{V} \quad (3-20)$$

Where P_{tot} is the total heater output power and V corresponds to the volume.

4. Chapter 4: Modelling and Simulation

4.1. Introduction

This chapter analyses how the system was modeled and simulated on Aspen plus®. A solid-based simulation on Aspen plus® was used for the development of the gasification model. This was done in order to accommodate waste plastic feedstock. Various assumptions were made to develop the model for the simulation of waste plastics gasification. The process model presented in this work is a steady-state model continuous gasification of waste plastic, simulated using Aspen plus® software (Advanced System for Process Engineering). The simulation of the process was described through an equilibrium-based, non-stoichiometric model. The model relies on experimental process conditions and feedstock composition detailed in chapter 5.

4.2. Process Modelling

4.2.1. Overview of Process Modelling

According to Omgamay (2020), the model simulations must imperatively predict the product over a range of process conditions. On Aspen plus® software, the user has the capability of building the proposed plant by inserting the process necessary information while using “blocks” to indicate calculation procedure in the software based on the user’s process parameters input. Furthermore, the software model is convenient and well adequate when conducting work with solids chemical processes. There are serious challenges presented by solids heat and mass balance calculations, that demand adequate physical property models that are fit for solids components (Aspentech, 2004). In addition, Aspen plus® software has at the user's disposal a vast and various database for both non-conventional and conventional and components. This makes it even more relevant for solid chemical processes simulation (Omgamay, 2020). Numerous studies on gasification models reveal that a steady-state model is the most convenient model for predicting the composition of gases and performing a sensitivity analysis on the process variables (Hlaba, 2020; Omgamay, 2020; Alembath, 2016 and Mavukwana, 2016).

A handful of researchers have conducted studies on waste plastics gasification. Al amoodi et al., (2013) developed a model on Aspen plus® to simulate Polyethylene gasification to predict the composition of the gasification products. Previous

investigations (Zheng et al., 2013; Ramzam et al., 2011) also demonstrated the effect of feedstock moisture content, air equivalence ratio, and gasification temperature on gasification performance. Even though a few studies have been conducted on waste plastic gasification particularly, literature report that heavy work has been conducted on gasification in general (Niksa, 2020; Li et al., 2020; and Bai et al., 2020) and it results from these studies that the most important parameters playing a vital role in gasification processes are the reactor temperature, the equivalence ratio, the steam-to-fuel ratio, the residence time and gasifying medium. In order to obtain a better reliable system, the operating parameters must be optimized and controlled with significant accuracy (Al amoodi et al., 2013).

4.2.2. Model Approach

The literature (Kannan, 2012) reveals that the gasification process models until far studied can be grouped into steady-state or quasi-steady-state, or transient state models. The group models which do not consider time as a derivative are the steady-state models. They are further classified as kinetic rate models or kinetic free equilibrium models (Paviet et al., 2009). The aforementioned models have been used by some researchers to conduct studies on modeling the gasification process for various fuels. Following is a list of these searchers and their work. Robinson and Luyben (2008) studied the transient model on coals. Nikop and Mahinpey (2008) addressed the steady-state kinetic model for biomass, and in 2006 Mastellone et al., used the steady-state kinetic model for waste plastic. The kinetic free equilibrium model for biomass was used by Doherty et al., 2009; Paviet et al., 2009; and Shen et al., 2008. Finally, Mitta et al., (2006) used the kinetic free equilibrium model on tires. From these models, the kinetic free equilibrium steady state is mostly preferred when predicting the temperature and the product gas composition. It is also the most preferred because of the sensitivity analysis of process parameters.

The Kinetic free equilibrium model is the model approach taken in this work to investigate the optimization of waste plastic gasification. This model approach corroborates with the work of Al Moody et al., (2013) as well as the work of Mitta et al., (2006) who respectively used kinetic free equilibrium to simulate the

gasification of polyethylene and the gasification of the waste tire. The advantage of such an approach is that, on one hand, it focuses only on the product equilibrium. Meaning hydrogen (H_2), water (H_2O), methane (CH_4), carbon dioxide (CO_2), nitrogen, and sulfurous compounds. On the other hand, the unlikeliness for other hydrocarbons like oils and tar to form under equilibrium is very high. Consequently, they are not incorporated in the process simulation. Another benefit is the fact that the equilibrium condition simplifies a thorough optimization study addressing key process parameters such as the equivalence ratio (ER), the steam – to-fuel ratio (S/F), the gasification temperature, and the gasifying medium, thus overlooking the complexities of the reaction kinetics and the gasifier hydrodynamics.

The manual titled “Getting started modeling processes with Solids” from Aspen plus® 2004 was used as a cornerstone to developing the essential operation of the model developed in this study. This above-mentioned manual described in detail the simulation model developed for the combustion process. Due to its vast database including thermodynamics, chemical, and physical data for a variety of chemical compound and thermodynamics models, Aspen plus® has the potential to simulate most industrial processes using blocks that are operating as reactors and any other unit operations (Zheng and Furimsky, 2003). Aspen plus®'s wide variety of chemical compounds and selection of thermodynamics models which are crucial for any accurate simulation of any given chemical system renders it very relevant for this work. The present work is adapted from the combustion of the coal simulation model obtained from the aforementioned manual on Aspen plus®. Consequently, this current modeling involves the following:

- Non-conventional solid components like Ash are defined.
- The identification and specification of a global stream class.
- The stream containing unconventional components is indicated.
- The building of a process flow using Aspen plus® defined blocks.
- The physical properties of non-conventional solid components are specified.
- The components required for gasification are added. This includes both conventional and unconventional components.

- The alteration of component characteristics in unit operation blocks and specification of unit operation models.
- Fortran blocks are defined. This occurs so that Fortran statements are used to control the steps/reactions during gasification (Aspentech, 2004).

4.2.3. Gasification Model Development Assumptions.

During the development of this simulation model of waste plastic, numerous assumptions were made. These made assumptions are similar to those considered by (Aspentech, 2004, Hlaba, 2020; Soka, 2020; Mitta et al.,2006 Begum et al., 2014, Chen, 2011, Deng et al., 2019, Mavukwana et al., 2013, Shaohua et al., 2012, Zheng et al., 2013) and are as follows:

- The simulation model is in a steady state.
- It is an isobaric, isothermal, and kinetic-free system.
- The state of equilibrium is the state at which the chemical reactions occurring in the gasifier take place.
- Except for sulfur, all other components present in the model, participate in the chemical reactions.
- In the solid phase, carbon and ash are the only elements that constitute the char residue.
- All gases including hydrogen (H₂), carbon monoxide (CO), carbon dioxide (CO₂), oxygen (O₂), nitrogen (N₂), and methane (CH₄) that are involved in the model simulation are considered ideal.

4.3. Process Simulation

4.3.1. Simulation Model Process Flow Diagram

Due to the solid aspect of the feedstock, a solid-based simulation approach was used on the simulation software, Aspen plus®. This was done so that the processing of waste plastics in pellets form can be accommodated. The reason behind this approach is the fact that the mass and energy balance simulation of a process incorporating solid, demands specific physical properties that are suited for solids components. This in return is due to the fact that physical property suited for the characterization of the liquid element may not be relevant when used on solid elements (Aspentech, 2004). The benefit of using specialized property

models for the processing of solids stands on its capacity to precisely characterize the solid particle size distribution which could be a fundamental component in solid processing (Hlaba, 2020). The process highlighted in figure 4.1 here below is an Aspen Process Flow Diagram of the RFD gasification.

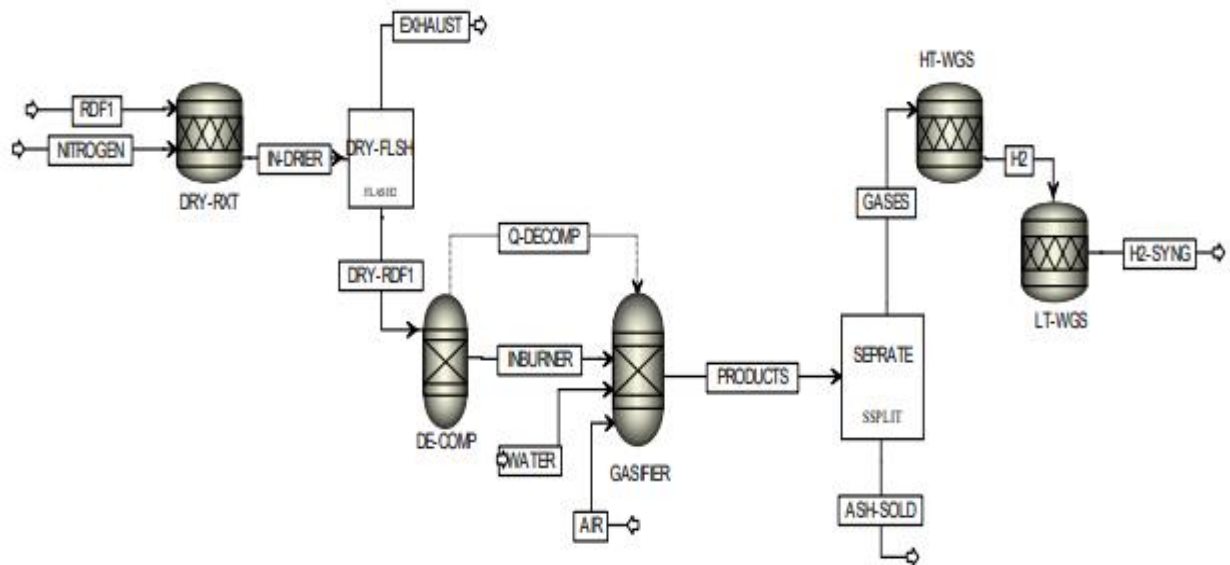


Figure 4-1: RFD Gasification Process Flow Diagram (Adefiso, 2018)

Despite the fact that the realistic gasification process takes place in a single unit or reaction container, the process is constituted of diverse steps which can be classified as process steps. There is no single unit operator block on Aspen plus® that acts as a gasifier. Hence, the development of process flow is fundamental in this work in order to model but also describe separately the stages that occurred in the course of this simulation. To perform each process step description and model in this simulation, a unit operator block corresponding to that process step is used. According to Kannan et al., (2012), the gasification process is divided into three process stages. Namely, the first stage is the drying, the second stage is the pyrolysis, and the third stage is gasification. In this gasification process, the feed used is waste plastic pellets, and it was identified in the model as a nonconventional element and specified in the simulation based on the ultimate and proximate analysis data obtained from Yao et al., (2018) and expressed in table 4-1 here below. The model is based on the minimization of Gibb's free energy at equilibrium, and it is assumed the residence time is adequately sufficient to allow the reactions to acquire the state of equilibrium (Hlaba, 2020).

Table 4-1: Proximate and Ultimate Analysis Data (Adapted from Yao et al., 2018)

Proximate Analysis %		Ultimate Analysis %	
Moisture Content (MC)	0.25	Carbon (C)	80.18
Fixed Carbon (FC)	0	Hydrogen (H)	14.84
Volatile Matter (VM)	94.77	Oxygen (O)	3.61
ASH	4.98	Nitrogen (N)	0.06
-		Sulfur (S)	0.08

4.3.2. Description of the Simulation Process

Three main unit blocks type of reactor was used on Aspen plus® software for the simulation of the current gasification process. These three main reactor types were the RGibbs reactors, the Stoichiometric Reactor (RStoich), and the Yield Reactor (Ryield).

4.3.2.1. Drying

The first step taking place in the gasification process is the drying stage. In this section of the process, the raw material is fed into the unit block and mostly heating and drying of particles are taking place. The RStoich type of reactor was used to simulate this drying stage. Indeed, despite the waste plastic pellets (feedstock) being dried already during its production, it still contains some amount of moisture. Hence during this stage of the process evaporation is taking place and the content in the moisture of the feedstock is reduced to its lowest. This moisture content is indicated through proximate analysis.

4.3.2.2. Pyrolysis/Decomposition

The second process step occurring in the gasification process is the pyrolysis also known as the decomposition stage. In this stage, the waste plastic is being decomposed into its different constituent components. The Ryield reactor is the type of unit block that was used to simulate this decomposition process. The basic principle behind this stage is that the Ryield reactor converts the non-conventional feed component into conventional components. In order to compute the yield distribution from the element characteristics, the Fortran statement was used in a calculator block. The result is obtained in a form of an elemental composition defined by the ultimate analysis of the feed stream.

4.3.2.3. Gasification

The third stage after the pyrolysis stage is the gasification step itself. The decomposition stage has just occurred and the initially nonconventional component has been converted into conventional elements and they are ready for gasification. These elements present in the outlet stream of the pyrolysis reactor are mixed with an external air stream. A mixer unit block was used to favor the perfect occurring of the mixing. This actual gasification stage is simulated using the RGibbs reactor model as previously indicated in section 4.3.2. The principle behind the RGibbs reactor model is that it rigorously calculates chemical and phase equilibrium while minimizing Gibbs free energy of the system. Thus, such a model does not necessarily require the specification of the reaction stoichiometry. The minimization and assumption of complete chemical equilibrium enable the reactor to compute the SYNGAS product stream.

4.3.3. Operating Process Parameters

The following parameters in the table below constitute the gasifiers operating parameters for the gasification process.

Table 4-2: Process Operating Parameters

Parameter	Unit	Value
Feed Flow rate	Kg/h	30
Feed Pressure	bar	1
Feed Temperature	°C	25
Air Equivalence ratio	-	0-1
Air Pressure	bar	1
Air Temperature	°C	25
Gasifier Pressure	bar	1
Gasifier temperature	°C	500-1300

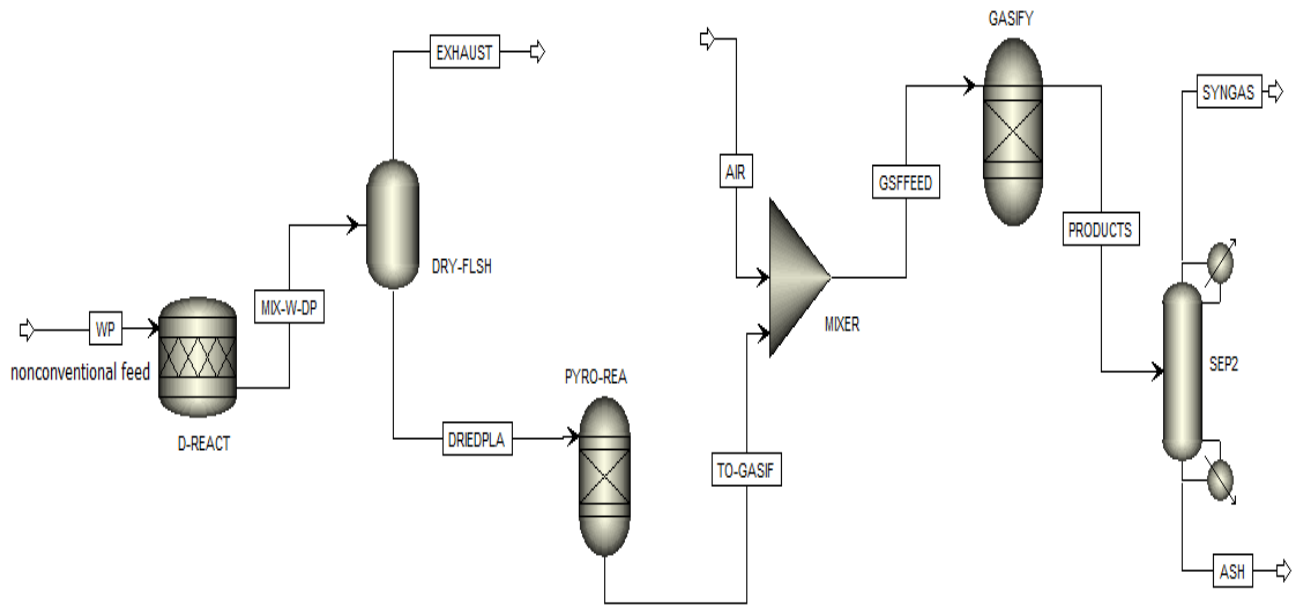


Figure 4-2: Waste Plastic Aspen plus® Flow Diagram representation

4.3.4. Sensitivity Analysis

In order to monitor the relationship between diverse parameters and the syngas composition, a sensitivity analysis was performed. In this current study, the temperature, the pressure, the gasifying agent both air flow and water flow rates are used so that their effects on the syngas produced can be evaluated.

4.4. Model Validation

The model was validated with literature experimental studies (Mavukwana., 2016 and Soka., 2020). The present experimental study and simulation results were compared to the work of Kannan et al.,2012 who performed a Process Optimisation of waste plastic gasification. The table below provides a comparison between this work and the work of Kannan et al. This section in order to be more in line with the current work, it would be further discussed in Chapter 6: Results and Discussion.

Table 4-3: Comparison: Aspen Simulation versus the experimental results

Product	Experimental Results (%) (Kannan et al., 2012)	Aspen Simulation (%)
Hydrogen (H₂)	35	39
Carbon Dioxide (CO₂)	8	17
Carbon Monoxide (CO)	25	34
Methane (CH₄)	3	10
Temperature	1000K	1000K

5. Chapter 5: Experimental System and Material Characterization

5.1. Introduction

In this chapter, the product of the gasification process is analyzed, and the model is validated.

5.2. System Setup and Experimental Procedure

5.2.1. System Setup

Figure 5-1. represents a schematic representation of the system setup. A 230V socket supplied an electric current to the IR reactor. The reactor is connected to four thermocouples that assist in setting each of the 4 ceramic heaters' temperatures. The gases are collected from the reactor in a Tedlar bag, then analysed using gas chromatography.

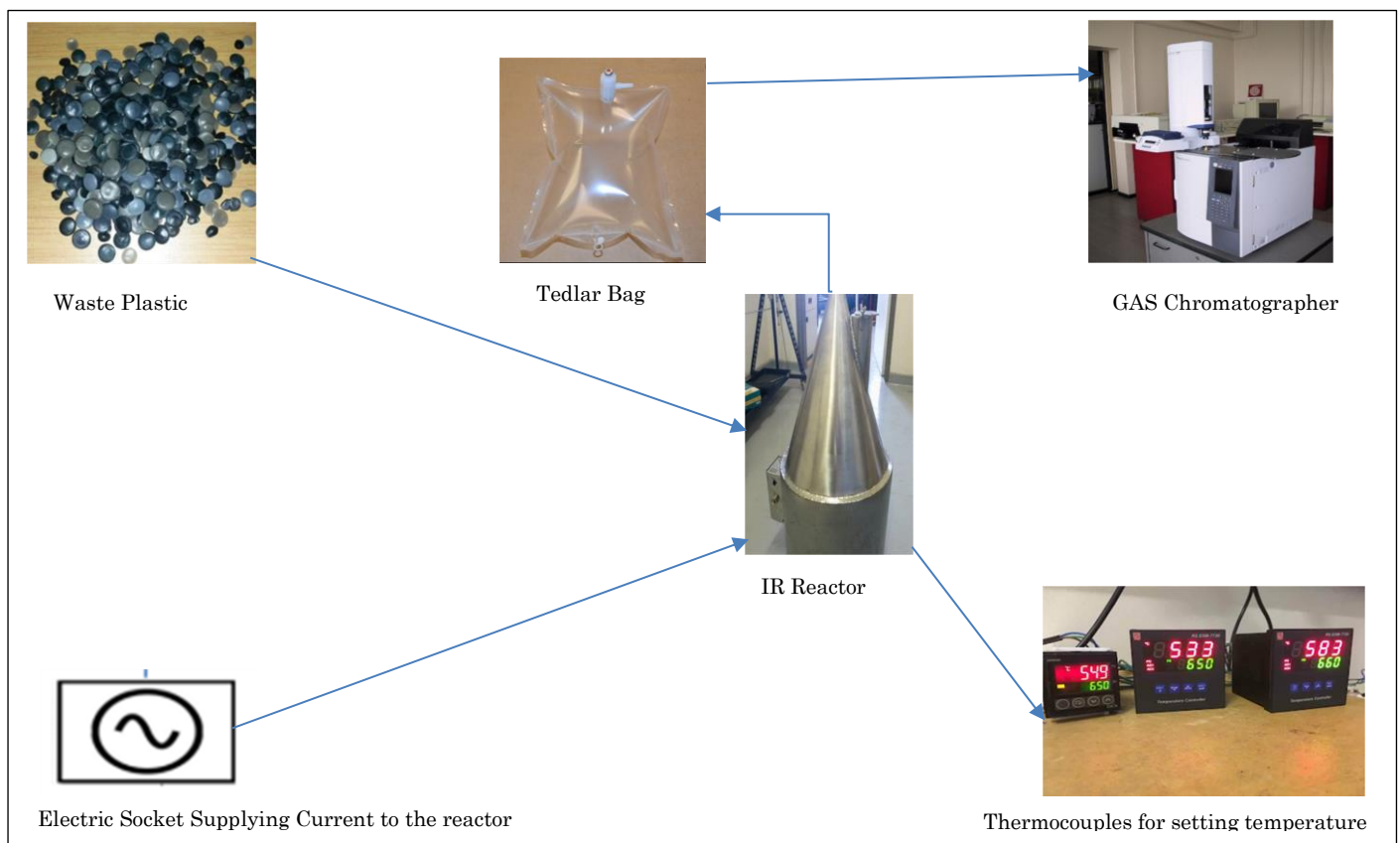


Figure 5-1: System Design Schematic

5.2.2. Experimental Procedure System Setup

- The reactor is preheated (250 to 300°C).
- A certain amount (20 to 30 grams) of waste plastic is pelletized
- The weighted pelletized waste plastic is placed in an open container.

- The then open container would be placed in the reactor
- The temperature would then be set to the optimum degree of 700°C
- After an hour gas samples would be collected and taken for further testing

5.2.3. Gas Chromatography

In this work, a compactGC^{4.0} (Global Analyser Solutions, Netherlands) was used for gas composition analysis. The product exiting the reactor system was collected and sent for analysis of hydrocarbon compounds (C₁ – C₆) and elements such as nitrogen (N₂), Hydrogen (H₂) Oxygen (O₂), Carbon dioxide (CO₂), and Carbon monoxide (CO).

The GC analysis of the gasification product reveals the presence of N₂, H₂, O₂, CO₂, CO. It also highlighted the presence of other gases such as C₃H₈, C₆H₁₄, and C₄H₁₀ in small quantity. The composition of the syngas obtained varied based on factors like pressure, temperature and parameters flow rate. The results of this experiment align with the work of He et al., (2009) who investigated Syngas production from catalytic gasification of waste polyethylene: Influence of temperature on gas yield and composition. This work is based on the hypothesis that the gasification of waste plastic is a process involving carbon-based elements and steam to generate syngas and minor hydrocarbon. Table 5-1 presents the predicted values obtained from the simulation of the model on Aspen Plus and the experimental results values. The analysis of table 5-1 showcases that experimental results are not close to predicted values. This is mainly due to the incapacity to maintain and control the gasifier temperature at 800 °C which was observed to adequate temperature for gasification. This would have avoided over heating of the heaters leading to their destruction during each experiment. Other causes could be the calibration or measurement errors that happened during the experimental runs.

Table 5-1: Comparison of Predicted values with experimental values.

Product	Predicted Values (%)(Simulation)	Experimental Values (%)(current study)
H₂	39	21.3
CO	34	5.7
CO₂	17	15.2
CH₄	10	0.2

5.3. Material Characterization

5.3.1. Thermal decomposition

The phenomenon of thermal decomposition of plastic can be described through a number of parallels or series of chemical reactions by chain scission mechanism or through random scission mechanism and several others (Saha et al., 2008). According to Toledo (2013), thermal analysis indicates a series of methods used to uncover the chemical or physical properties of an element while kept at a constant temperature, heated, or cooled.

Thermogravimetric analysis (TGA), Fourier Transform Infrared Spectrometry analysis (FTIR), and Differential Scanning Calorimetry analysis (DSC) on our samples were all performed at Cocosolutions Technology (Pty) Ltd where PerkinElmer© STA6000 was used for DSC. As for the FTIR, a Spectrum 3 MIR/NIR/FIR Spectrometer (PerkinElmer, USA) was used. The results are shown in figures 5-2, to 5-4 for DSC and FTIR respectively.

5.3.2. Differential Scanning Calorimetry (DSC)

Differential Scanning Calorimetry (DSC) measures the change of the difference in heat flow rate to a sample and its reference while both undergo a temperature-controlled program (Höhne et al., 2013). The DSC assesses the property change such as the heat flow rate difference. Typically, temperature alteration of the sample is the cause of heat flow rate difference. Figure 5-2 indicates the DSC of HDPE and LDPE. The curve expresses the heat flow versus the temperature. It can be seen from the graph that the peak temperatures are 132.2 and 124.5 °C for HDPE and LDPE respectively. This could be an indication

of the exothermic reactions taking place. The change in phase of the graph could further indicate a transition taking place at that temperature. This transition could be the melting of the material.

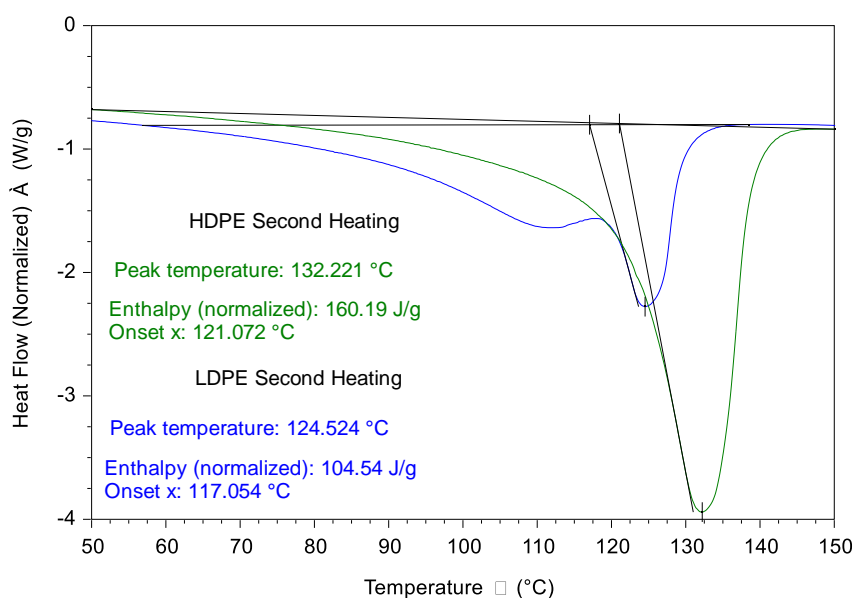


Figure 5-2: Differential Scanning Calorimetry Schematic

5.3.3. Thermogravimetric Analysis (TGA)

The measurement of sample weight, based on their temperature is defined as Thermogravimetric Analysis (TGA). The thermogravimetric analysis shows sample decomposition behavior during heating. It detects the gain or loss of a mass of a sample and evaluates stages by stages the changes in mass. This process is represented as a percentage of the initial mass. Subsequently, the temperature that characterizes a stage in mass loss or mass gain is determined by TGA. A sample weighing 3mg was placed on a ceramic pan. The ceramic pan was then heated with the PerkinElmer TGA, starting from 150°C to 550°C. The temperature change was operated at a rate of 5 to 10°C /min. This temperature rate change was obtained from Ali, and Qureshi (2011) study, based on Catalyzed pyrolysis of plastics: A thermogravimetric study. The current TGA primarily serves as an assessment to waste plastic characterization. Figure 5-3 shows the TGA results generated on waste plastic. The plot shows the percent mass as a function of sample temperature for the waste plastic under a nitrogen purge. The TGA results show that waste plastic start undergoing thermal degradation at 379.6°C and end

at 417.3 °C with a total mass loss of 99.1%. The constant degradation behavior observed in Figure 5-3 at corresponding ranging temperatures is a characteristic of HDPE and LDPE which are types of plastics (Oyedun, et al., 2014).

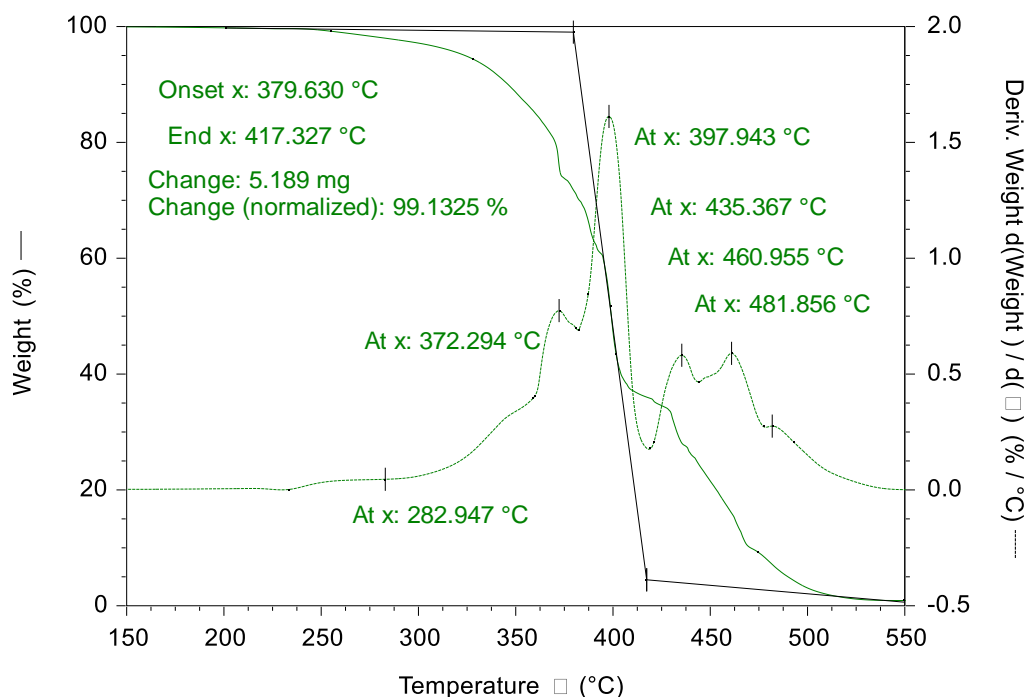


Figure 5-3: Thermogravimetric graph

5.3.4. Fourier Transform Infrared Spectrometry (FTIR)

Fourier Transform Infrared Spectrometry (FTIR) is used to identify organic and inorganic materials. Radiation is passed through a sample and the portion of the incident radiation that passed through particular energy and is absorbed will constitute the infrared spectrum (Stuart, 2004; Patz et al., 2004). The FTIR is based on the attenuated total reflection (ATR) technique for the characterization of materials. The protocol for this technique is based on a non-destructive approach since the material does not require to be dissolved or ground before being tested. The confirmation of the sample is done by carrying out a comparison of a particular region of the wavelength peaks to another reference spectrum that constitutes the database. The spectrum resulting from this comparison will indicate the transformation and absorption which defines the molecular fingerprint of the studied sample. In the case of a match in resulting peaks, a report is established. In the case of non-matching resulting peaks, the ATR analysis is automatically reported as inconclusive. Figure 5-4 represents the graph

of the FTIR analysis. The graph expresses the transmittance (%) versus wavenumber (cm^{-1}). It can be seen from the FTIR graph that at the wavenumber of 2970 cm^{-1} , HDPE has a transmittance of 72% and LDPE a transmittance of 55%. The analysis of figure 5-4 further reveals that at a wavenumber above 3500 cm^{-1} , HDPE and LDPE have a transmittance of 101 cm^{-1} . These values correspond with component libraries that are characteristics of plastics.

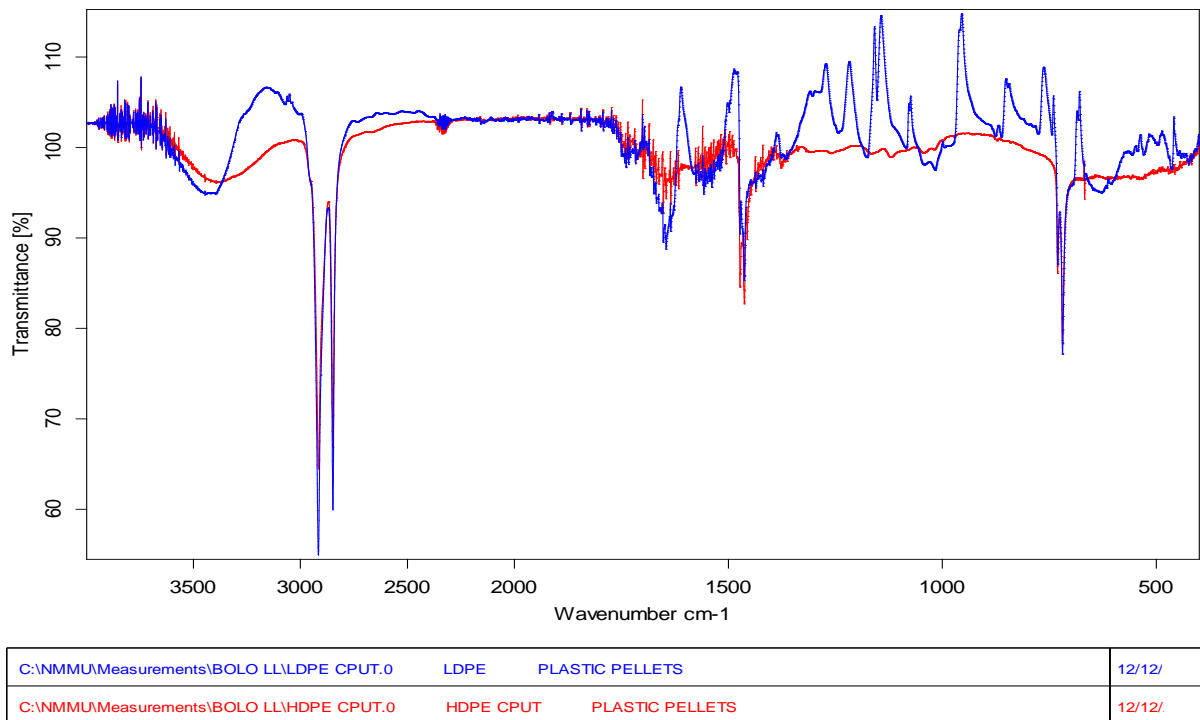


Figure 5-4: Fourier Transform Infrared Spectrometry

6. Chapter 6: Results and Discussion

6.1. Introduction

This chapter addresses the results of the simulation and those of the experimental system. It analyses the outcomes of this study and discusses the relevance of those outcomes. The primary element or result to be analyzed in this chapter is the simulation results. Through a sensitivity analysis, simulation results were obtained for certain parameters such as the temperature, pressure, airflow as well as the water flow.

6.2. Modeling and Simulation Results.

6.2.1. The Effect of Temperature on the Syngas Production

Temperature is a crucial parameter in the gasification process. In this study, the gasifier temperature was set to vary between 600-1300°C. Figure 6.1 below represents the outcomes from the Aspen plus® simulation. In studying the effect of gasifier temperature on syngas production, it was revealed that hydrogen (H₂) and carbon monoxide (CO) increments are proportional to the temperature increase as indicated in figure 6-1 below.

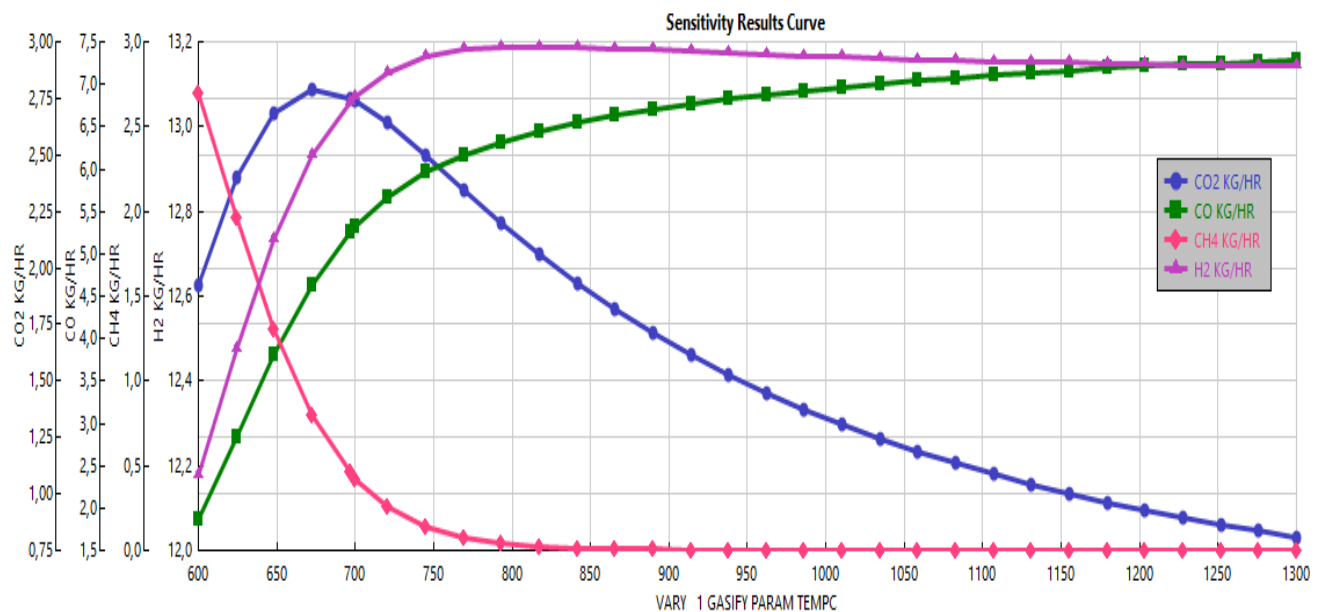


Figure 6-1: Effect of the Gasifier Temperature

The graph also indicates that while the temperature in the gasifier increases, the methane (CH₄) and carbon dioxide (CO₂) content decreases. It can also be seen that around 850°C the hydrogen content starts to slightly decrease

while the carbon monoxide keeps increasing. Eventually, the two trends (H_2 and CO) reached a ratio of 1 between $1200^\circ C$ and $1300^\circ C$. It is important to note that each element present in this graph is represented on its own separate scale and despite the fact that the graph indicates an intersection, this does not necessarily translate into equal value at those intersections. The interpretations that emanate from these results are a decrease in methane (CH_4) and carbon dioxide (CO_2) concentrations and a contrasting increase in hydrogen (H_2) and carbon monoxide (CO) concentrations. These can be attributed to two reactions, namely, carbon dioxide reforming as well as the exothermic steam methane reforming. This analysis correlates with the work of Mitta et al (2006) who investigated the Modeling and simulation of a tyre gasification plant for synthesis gas production and found out there were increase in hydrogen from 7-27% and carbon monoxide from 3-12% while there was decrease in methane and carbon dioxide respectively from 16-7% and from 22-12%. These observations are also corroborated by results presented by Deng et al (2019) who showed that an increase in H_2 , CO, and decrease in CH_4 , CO_2 could be explained by the “Le Chatelier principle”. This principle is also known as the Equilibrium Law states that if a system undergoes disturbance based on its temperature, concentration, or pressure, the system will respond to restore a new equilibrium state. Indeed, according to Deng et al (2019), the CH_4 and CO_2 reforming reactions are preventing since they are exothermic while H_2 and CO reactions are encouraged since they are endothermic reactions.

The graph below (Figure 6-2) indicates the percentage composition of syngas obtained. From the graph, it can be seen that the hydrogen content is the highest at 39% followed by the carbon monoxide at 34%, and finally the carbon dioxide and methane at 17% and 10% respectively. These varying percentages of the gasification products are essentially caused by the decomposition of char and the secondary reaction of the tar vapor as temperature increased, more steam and carbon is converted into gas following Boudouard, water-gas shift, and endothermic reactions. Hence, the steam decomposition and the carbon conversion efficiency increased consequently char reduced. This syngas components variation could also be based on the more favorable steam reforming and thermal cracking reactions at elevated temperatures, which resulted in the secondary cracking reactions into

the gas fraction. These results obtained are highly favorable if used as feedstock for Fischer-Tropsch synthesis for the production of transportation fuels. These results are validated by He et al., (2009), who investigated the syngas production from catalytic gasification of waste polyethylene and reported H₂ 36.92%, CO 27.37%, CO₂ 20.78% and CH₄ 9.94%. He et al observed that the syngas products increased with decrease char and liquids yields and, further observed that the higher temperature resulted in more hydrogen and carbon monoxide production.

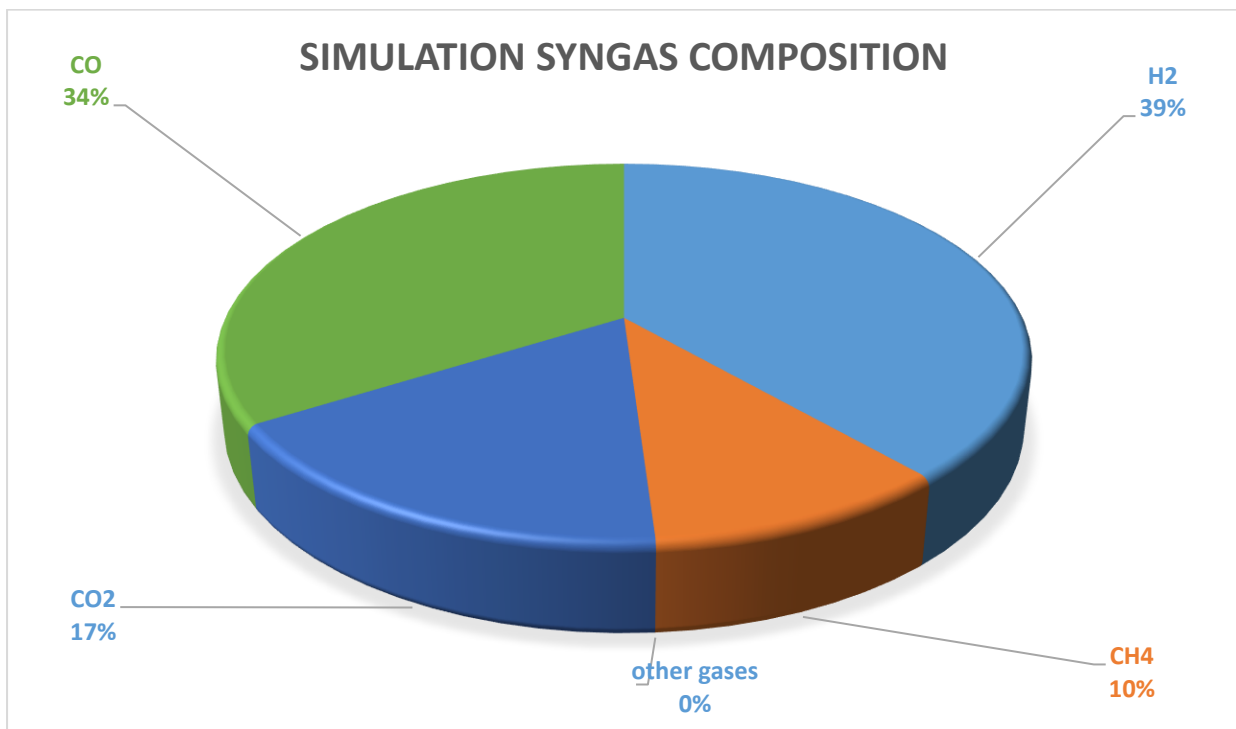


Figure 6-2: Composition of gas produced (syngas) from the model.

6.2.2. The effect of Gasifier pressure on Syngas composition

The pressure is another important characteristic of the gasification process in general. Figure 6-3 here below presents, a sensitivity analysis of the pressure effect on syngas composition. The gasifier sensitivity analysis pressure was set between 1-10 bar. This sensitivity analysis reflects that there is a steady increase in methane (CH₄) content as the pressure rises, while the rest of the syngas composition namely carbon monoxide (CO), hydrogen (H₂), and carbon dioxide (CO₂) all have a steady decrease. This result is in good agreement with the work of Mishra et al., (2018) who reported that the pressure increase had an effect of upsurge on CH₄ content. This proportionality relation between the CH₄ surge and

the pressure rise could be due to the secondary cracking taking place during the pyrolysis or decomposition step. This second cracking lead to rapid hydro-gasification.

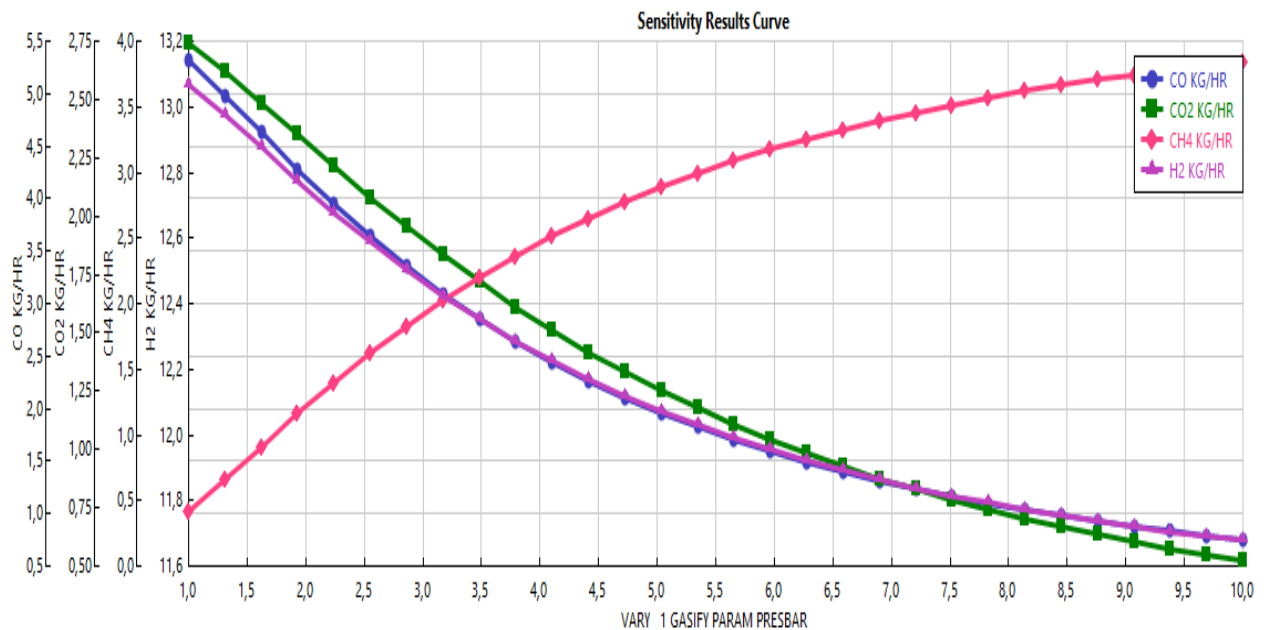


Figure 6-3: the pressure effect on syngas composition

6.2.3. The effect of Airflow rate on Syngas Composition

During a gasification process, various gasifying agents can be used. In this simulation analysis, the effect of those gasifying agents on the syngas composition was determined and this is what it resulted.

Pertaining to the relationship between syngas composition and airflow rate, figure 6-4 shows the effect of that gasifying agent on the syngas composition. It can be observed from the graph that as the flow rate of air increases, so those the content of CO and CO₂. The other remark that can be made in regard to this graph is that while the airflow rate surges, the CH₄ and H₂ content reduce. If it can be noted that CO₂ has a linear increase, on one hand, the remaining gases all have a hyperbolic increase (CO) or decrease (H₂ and CH₄). The interpretation that originates from these observations is that the growth in CO₂ and CO is the result of the oxygen that the gasifying agent (AIR) brings into the system. This results in favoring the production of CO and CO₂. This view aligns with Hlaba (2020) who studied the effect of airflow on corn starch through gasification. Hlaba showed increase in CO and CO₂ content in syngas composition. The airflow increase was

attributable to the carbon conversion. Otherwise stated this increase is due to the combustion taking place since it can be observed that the increase takes its origin from the value of 0 kmol/h. This means as the gasification process starts so is the carbon conversion.

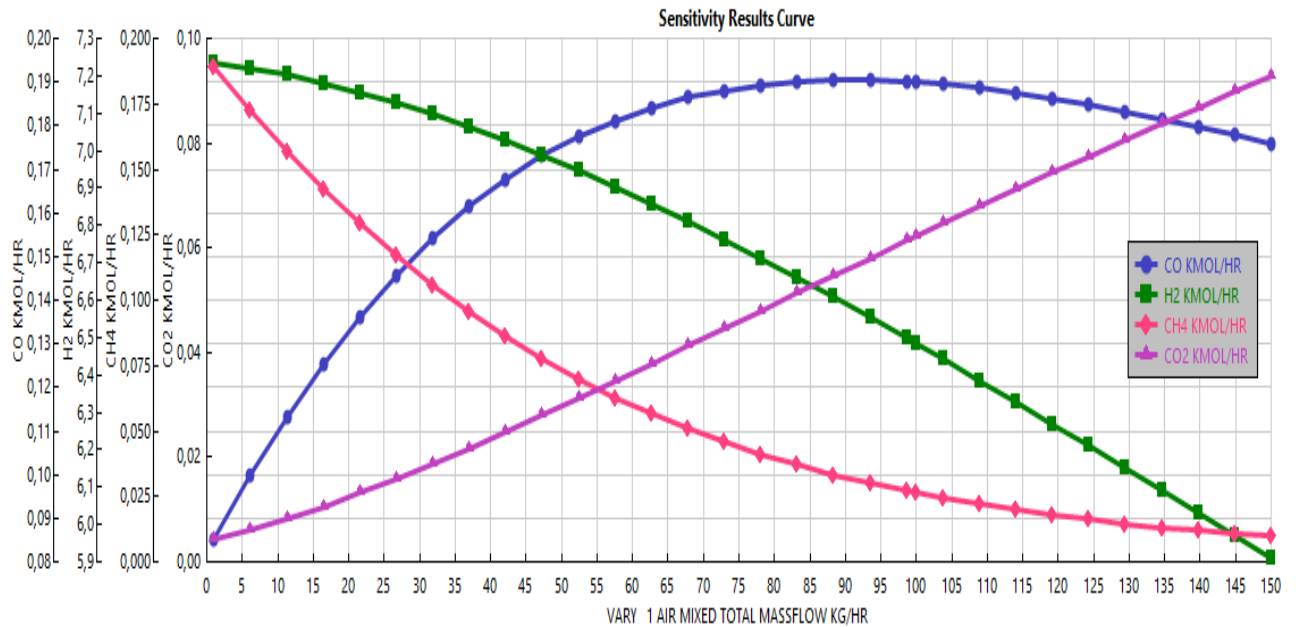


Figure 6-4: Effect of Airflow on syngas composition from waste plastic gasification

6.2.4. The Effect of water flow rate on the Syngas composition

This time around the gasifying agent used is water. The graph reveals an inversely proportional relation between the 4 constituents. This means as the content of hydrogen (H₂) and carbon dioxide (CO₂) increases, the content of methane (CH₄) and carbon monoxide reduces. It is also important to notice that the increase in both H₂ and CO₂ operates at the same rate throughout all the water flowrate. This means from 5-100 kmol/h. Primarily, it was expected that there would be an increase in hydrogen (H₂) and carbon monoxide content since the water-gas shift reaction is taking place here. The reason behind this analysis is based on the reactions which take place during the gasification process. In the current case, the reaction which should be favor is the water gas reaction. But since that did not take place and instead, the carbon dioxide and hydrogen content directly increased, it can only be deduced that in this case, scenario water is in excess, hence leading directly to the formation of CO₂ and H₂ thus their content proliferation. This view is similar to that of Deng et al., (2019) who studied the Simulation analysis of municipal solid waste pyrolysis and gasification based on Aspen plus®. They revealed that the upturn in CO₂ and H₂ instead of CO and H₂ during the increase in the gasifying agent (water) was due to its presence in excess.

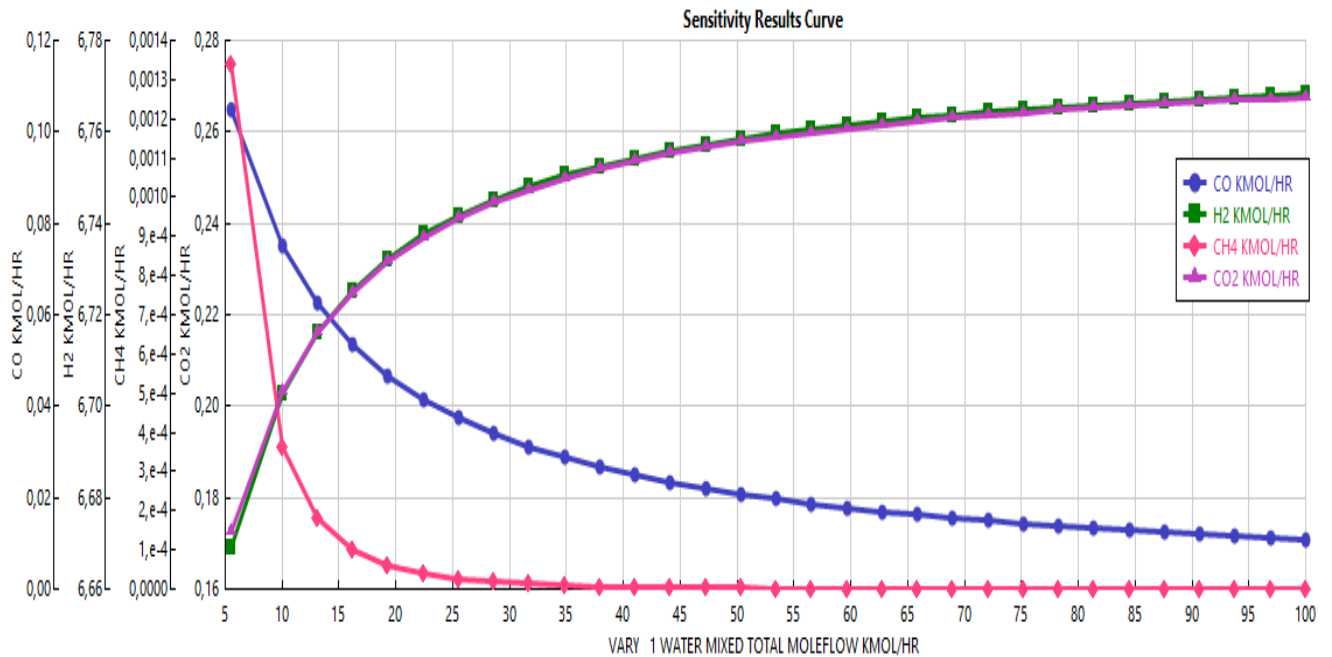


Figure 6-5: Effect of water flow in the syngas composition.

6.3. Experimental and Model Results analysis

The gas chromatography analysis conducted in the lab also revealed the presence of other gases such as C_3H_8 , C_6H_{14} , and C_4H_{10} . The presence of these longer-chained hydrocarbons could be interpreted as an incompleteness of the pyrolysis process. Despite the fact that such gases are to be expected, literature (Soka, 2020) revealed that they are usually in trace and sometimes undetected by the GC analysis. In order to further attest to this hypothesis, a sensitivity analysis was conducted on the Ryield reactor where the pyrolysis is taking. This analysis confirms the hypothesis and aligns with Soka, (2020) work. Soka performed a model and simulation on corn-starch and after performing a GC analysis Soka found the presence of other gases such as butane (C_4H_{10}) Propane (C_3H_8) and hexane (C_6H_{14}). He performed a sensitivity analysis and realized that the GC results and the Ryield sensitivity analysis results had the same trend. This means a sharp increase and when it reached the 500°C temperature it started steadily to decrease. In other words, the combustion has reached its completion.

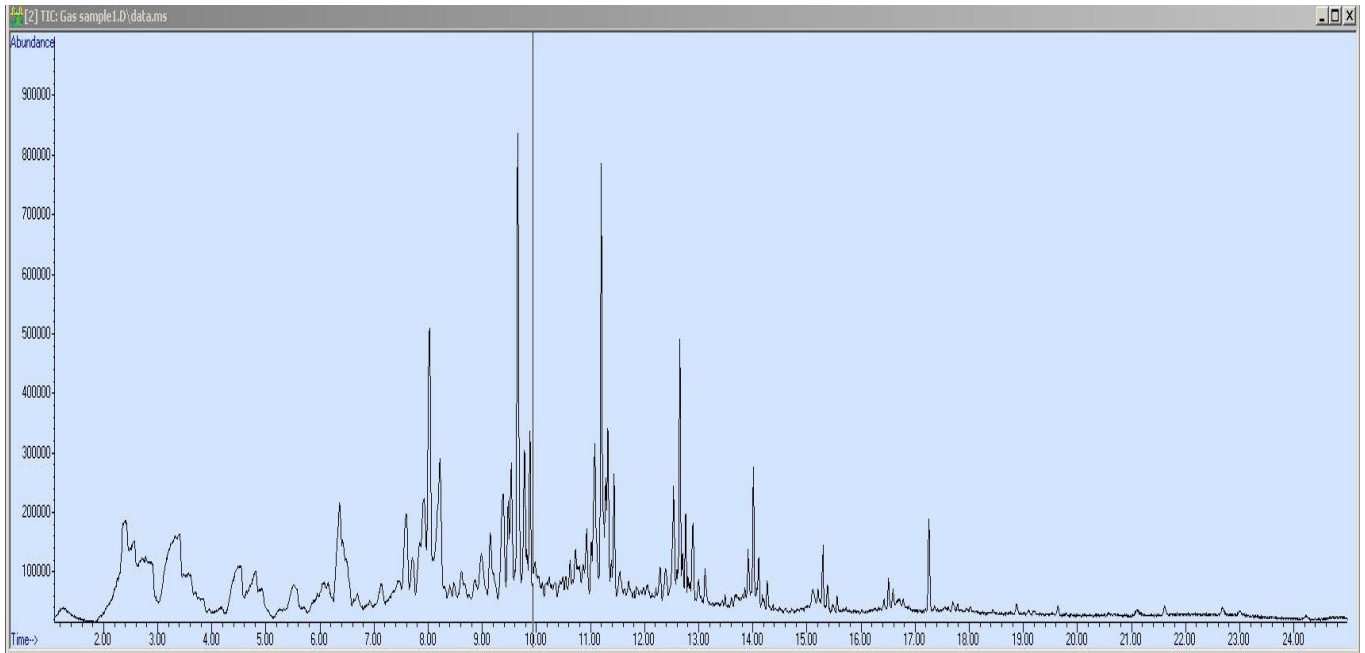


Figure 6-6: GC analysis

Even though the GC analysis also indicates the presence of other gases, which could be due to an inadequate during the experimental run in the laboratory, which in return led to uncertainty as to whether the equilibrium was reached during the experiments, the model provides a good prediction of hydrogen, Carbon monoxide, Carbon dioxide, and Methane. This means that this model could be adopted to predict products in the event of unnecessary laboratory works.

6.4. Discussion

The main objective of this research work was to optimize the production of syngas from waste plastic gasification. A two-approach study was performed in order to meet that objective. Based on the obtained results in the previous section of this chapter, the optimum parameters for syngas production are around 790-840°C for the temperature and 1bar for the pressure.

As for the flowrate, results reveal that the water flowrate had a bigger effect on syngas production than the air flowrate. The optimum syngas when alternating the water flowrate was between 75-100 kmol/hr.

The experimental study analysis revealed that the presence of gases such as Propane, Butane, and Hexane. This is the result of an incomplete combustion

taking place in the reactor. Even though the experimental study did not reveal to a good degree the expected results, the modeling, and simulation in return portrait an excellent trend with previous studies in the literature.

7. Chapter 7: Conclusion and Recommendations

7.1. Conclusion

The energy crisis added to the environmental pollution are two eminent challenges that the human species would be faced with if nothing is done to address them. This work aims at providing the beginning of solutions to these two challenges. By first addressing the pollution of the environment with plastic waste and secondly by attempting to generate energy source out that waste plastic. Hence the study carried out in this work is the Process Optimization of Syngas Production from Gasification of Waste Plastic using a Small Scale IR Reactor.

The question that this research project aimed to solve was to determine the optimum parameters of syngas from waste plastic gasification in a small IR reactor. The problems investigated were therefore divided into sub-problems, including the following:

- Design a reactor gasifier with infrared that would be used as a furnace for the gasification of waste plastic.
- Model and simulation using Aspen Plus to investigate the optimum parameters such as Temperature, Pressure, Air Flow, and water Flow rate.
- An experiment to be performed to validate the model.

7.1.1. Design a reactor gasifier with infrared heaters that be used as a furnace for the waste plastic gasification process.

A review was performed in order to obtain mathematical model expressions used for this research. A system was designed and material characterization was performed in order to determine structure and properties. The system designed described a proof of concept of the gasifier for plastic waste gasification.

7.1.2. Model and simulation using Aspen Plus to investigate the optimum parameters such as Temperature, Pressure, Air Flow, and water Flow rate.

Grounded on the work conducted, the results obtained and the analysis made, the pressure increase favors the methane content rise in Syngas. This was best

reflected at a pressure ranging between 1-10 bar. While the methane content rises due to pressure increase, on the other side the Carbon Dioxide, Hydrogen, and Carbon Monoxide content decrease. Furthermore, on the work conducted, the results obtained and the analysis made, the temperature at which the Syngas production is optimum appears to be ranging between 790 - 840°C. At that interval, the model reveals syngas content of 39% Hydrogen, 32% Carbon Monoxide, 17% Carbon Dioxide, and 10% Methane. Pertaining to the flow rate parameters, water flowrate appears to generate more Syngas when altering in comparison to the airflow rate.

7.1.3. Experiment performed to validate the model.

In regard to the experimental studies they did not concord with simulation and modeling results, however, were in agreement with the literature. The reason behind the non-concordance with simulations and modeling studies could be attributed to various inadequate such as poor GC calibration, equilibrium inadequate during experiments run, and incapacity to determine if equilibrium was reached or not.

7.2. Recommendations and Future Work

This work aims at optimizing syngas production hence based on the current study and research findings, the following work can be undertaken.

1. Conduct an experimental study based on the modeling and simulation of this current work, to attest and verify that the recommended running condition is feasible.
2. Conduct a full study both experimental and simulated on hydrogen production and optimization.
3. Conduct a study of the hydrogen with gas turbine and test for electricity generation.
4. Perform a quality analysis and application of the syngas of the developed system.

8. Appendix:

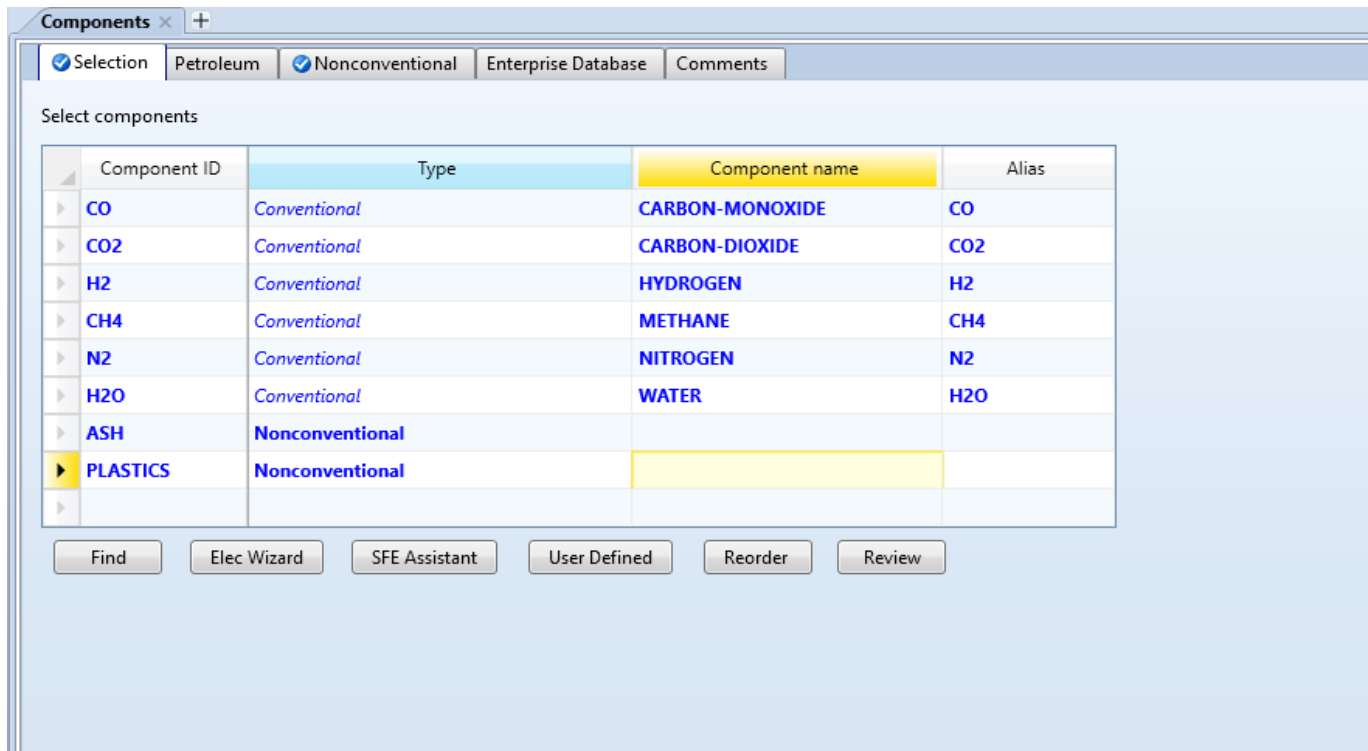


Figure 8-1 : Miscellaneous Figures Related To The Study

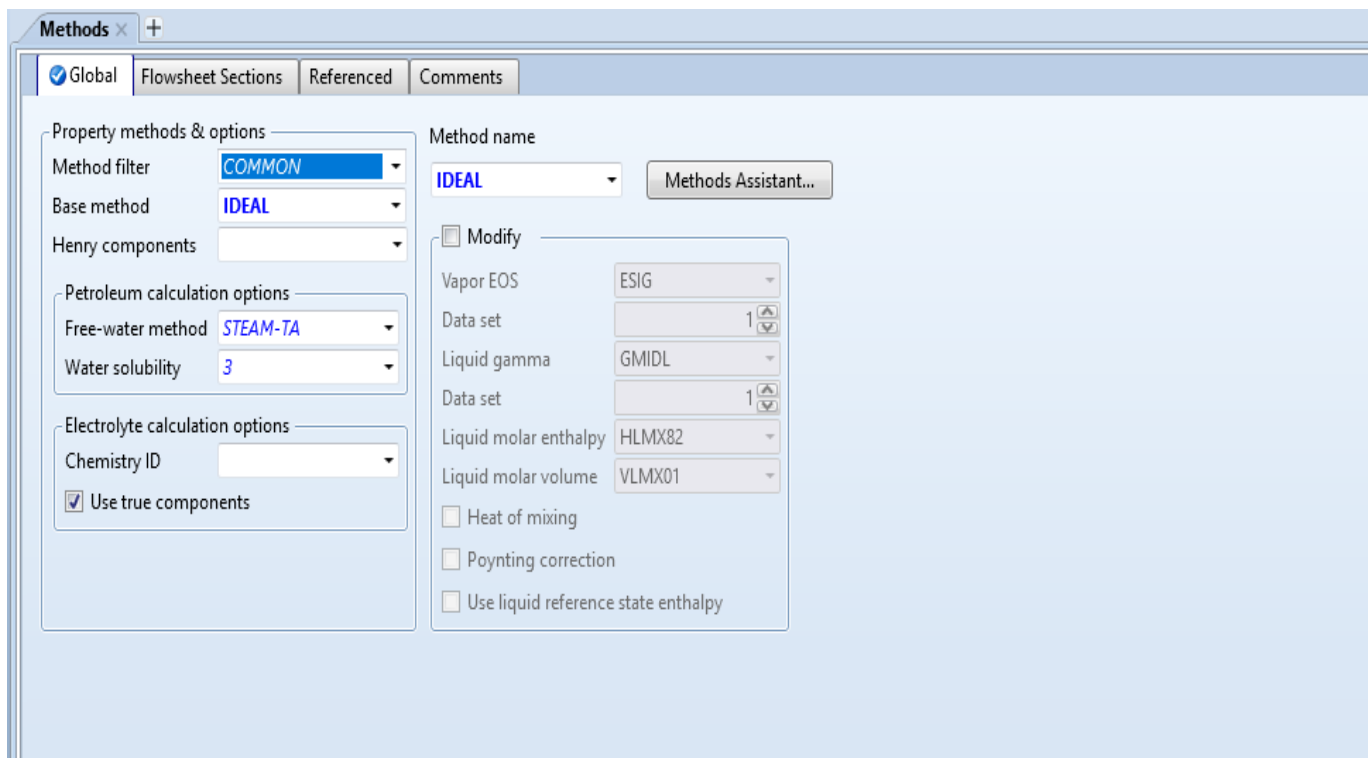


Figure 8-2: Method Selection

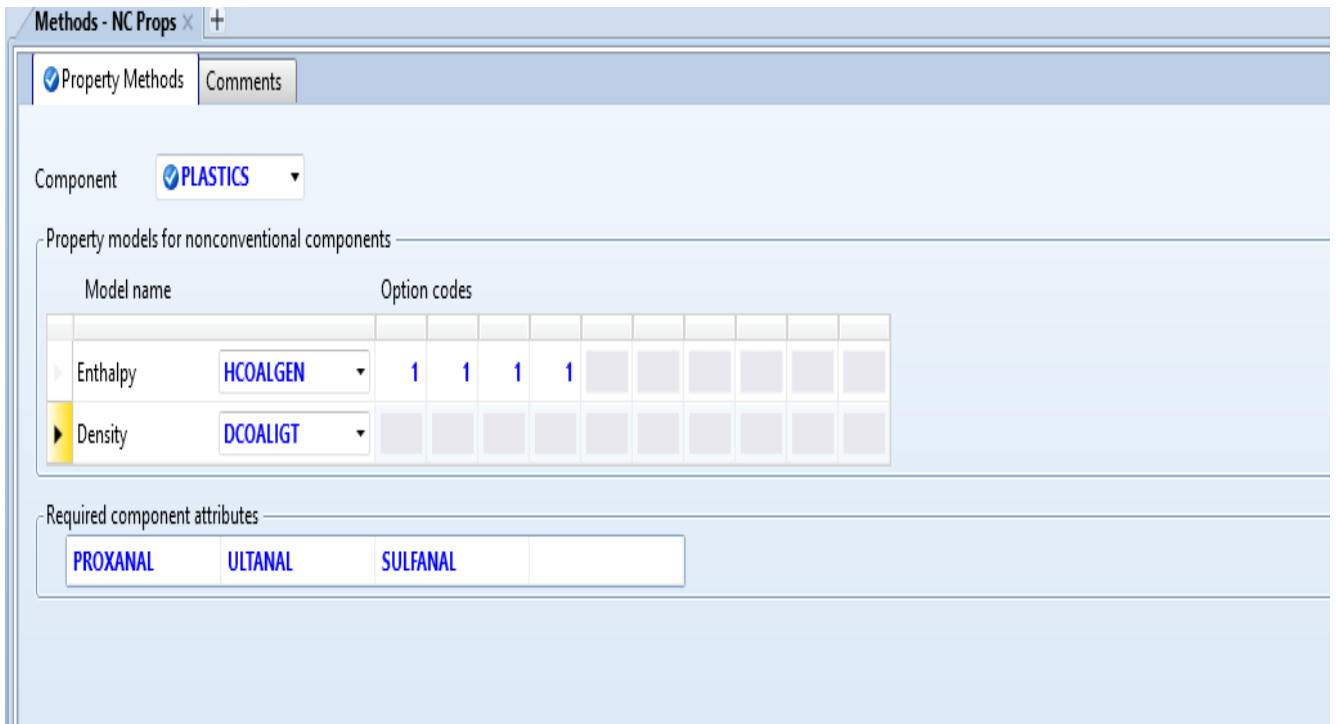


Figure 8-3: Property Methods Selection

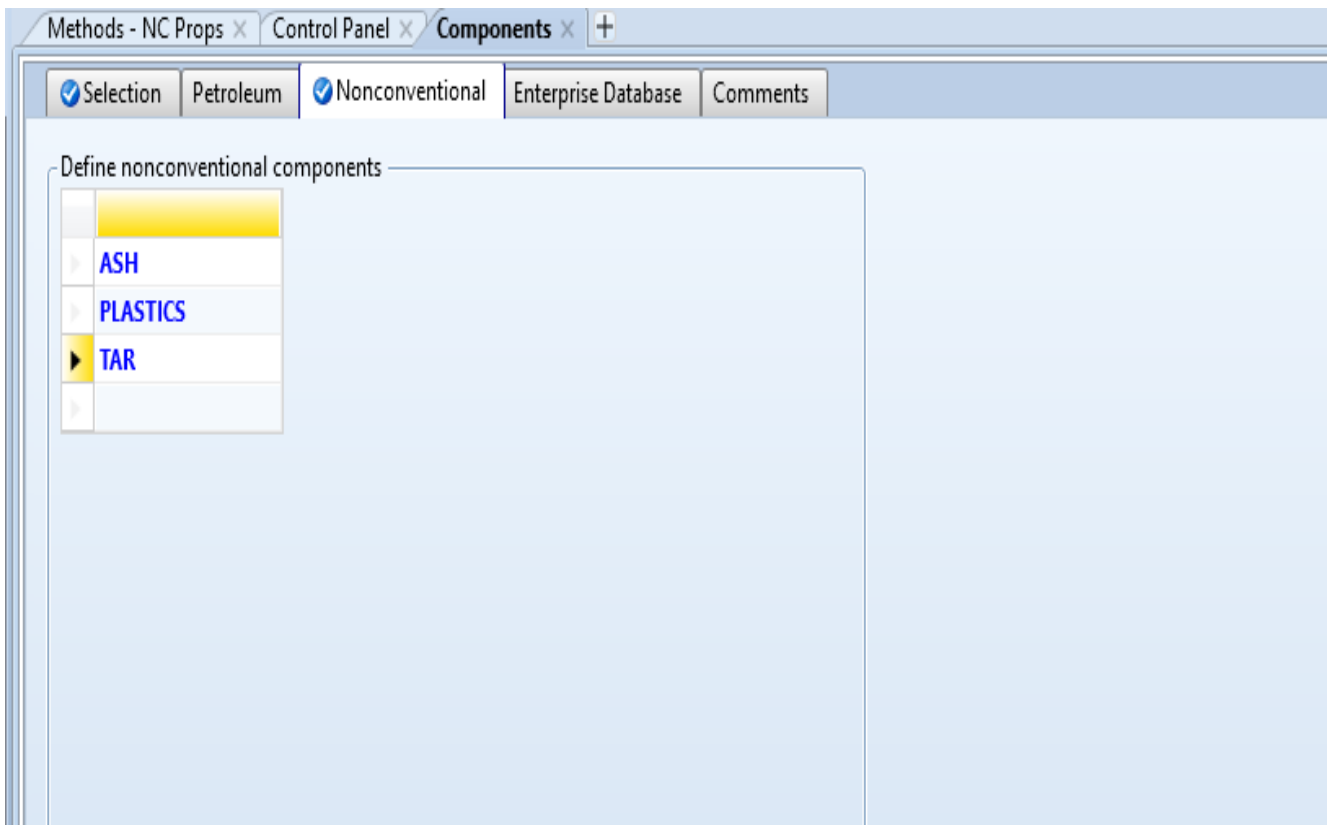


Figure 8-4: Nonconventional Components Setting

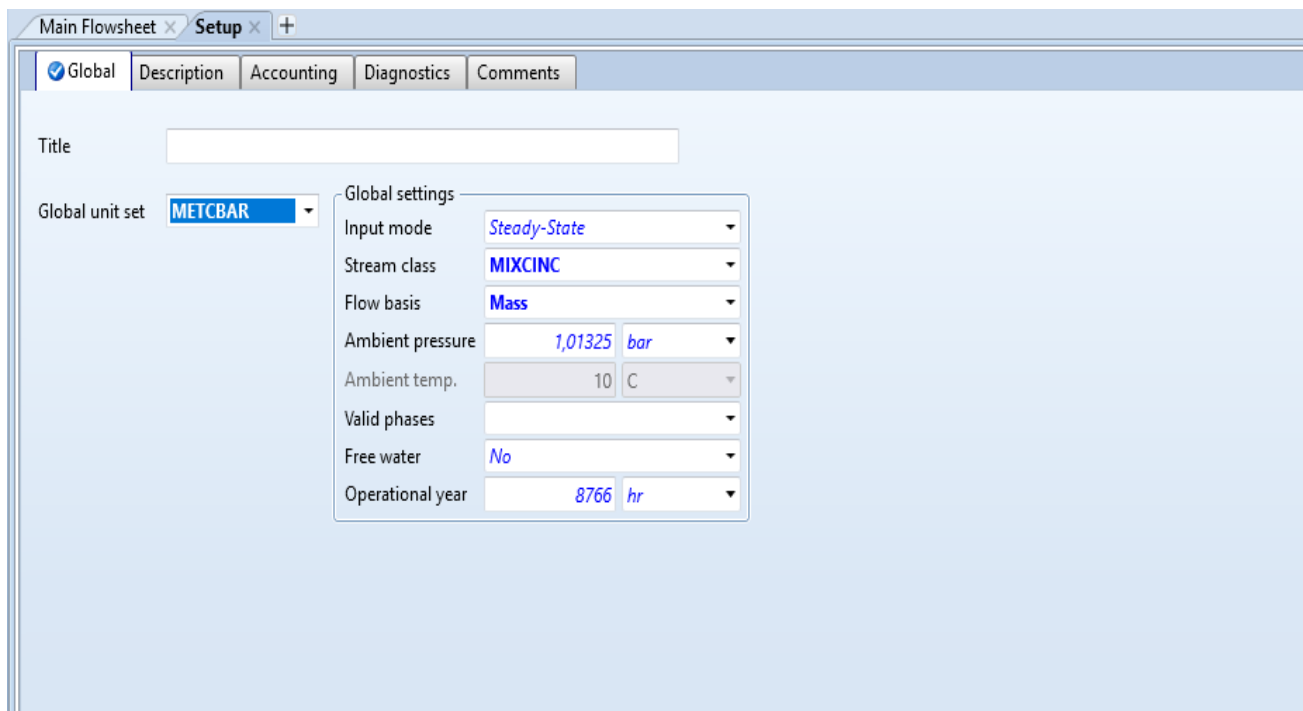


Figure 8-5: Stream Class Selection

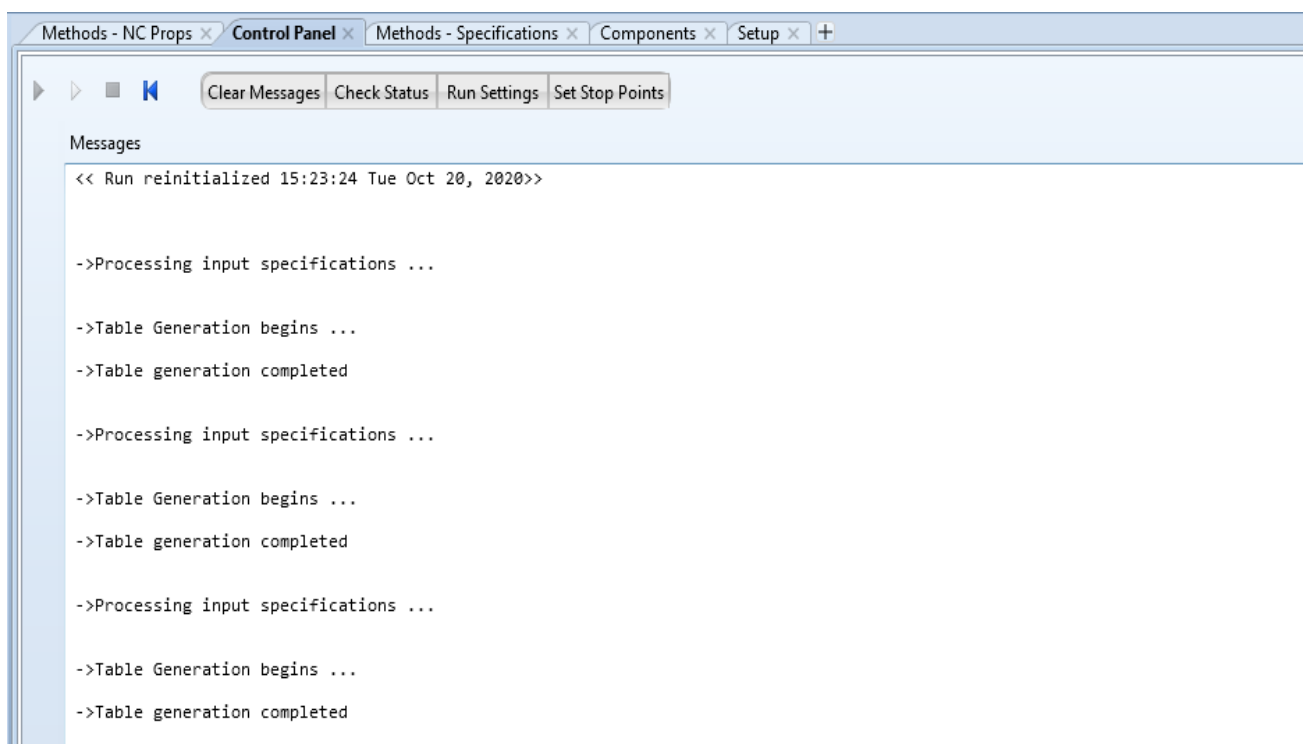


Figure 8-6: System Setup Feedback



Figure 8-7: Thermocouple Illustrating set Temperature.



Figure 8-8: Ceramic Heaters Mounted on the reactor

Table 8-1: Simulation Results

Material				
Stream Name	Units	GSFFEED	PRODUCTS	SYNGAS
Description				
From		B4	B5	B6
To		B5	B6	
Stream Class		MIXCINC	MIXCINC	MIXCINC
Maximum Relative Error				
Cost Flow	\$/hr			
Total Stream				
Temperature	C	276 664	700	700
Pressure	bar	1	1	1
Mass Vapor Fraction		1	1	1
Mass Liquid Fraction		0	0	0
Mass Solid Fraction		0	0	0
Mass Enthalpy	cal/gm	-453 678	-431 901	198 504
Mass Density	gm/cc	0,00031991	0,000194647	0,000126331
Enthalpy Flow	cal/sec	-156 267	-14876,6	2499,58
Mass Flows	kg/hr	124	124	453 314
CO	kg/hr	119 255	831 733	686 819
H2O	kg/hr	0,89441	216 433	184 535
CH4	kg/hr	0,745342	0,189757	0,050195
CO2	kg/hr	0,447205	764 042	0,0229213
N2	kg/hr	792 981	792 981	304 712
H2	kg/hr	89 441	676 195	603 705
O2	kg/hr	215 963	4,82E-15	0
S	kg/hr	0,149068	0,149068	0,03655
PLASTIC	kg/hr	0	0	0
ASH	kg/hr	0	0	0
Mass Fractions				
CO		0,0961731	0,0670752	0,151511
H ₂ O		0,00721298	0,174543	0,040708
CH ₄		0,00601082	0,0015303	0,00110729
CO ₂		0,00360649	0,0616163	0,000505637
N ₂		0,639501	0,639501	0,672186
H ₂		0,0721298	0,0545319	0,133176
O ₂		0,174163	3,88E-17	0
S		0,00120216	0,00120216	0,000806284
PLASTIC		0	0	0
ASH		0	0	0
Volume Flow	l/min			

MIXED Substream				
Phase		Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	276 664	700	700
Pressure	bar	1	1	1
Molar Vapor Fraction		1	1	1
Molar Liquid Fraction		0	0	0
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		1	1	1
Mass Liquid Fraction		0	0	0
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	-663 467	-6802,05	2029,01
Mass Enthalpy	cal/gm	-453 678	-431 901	198 504
Molar Entropy	cal/mol-K	748 836	104 669	110 846
Mass Entropy	cal/gm-K	0,512054	0,664602	108 443
Molar Density	mol/cc	2,19E+00	1,24E+00	1,24E+00
Mass Density	gm/cc	0,00031991	0,000194647	0,000126331
Enthalpy Flow	cal/sec	-156 267	-14876,6	2499,58
Average MW		146 242	157 491	102 215
Mole Flows	kmol/hr	847 911	787 347	44 349
CO	kmol/hr	0,425751	0,296937	0,245202
H ₂ O	kmol/hr	0,0496473	120 139	0,102433
CH ₄	kmol/hr	0,0464597	0,0118282	0,00312883
CO ₂	kmol/hr	0,0101615	0,173607	0,000520822
N ₂	kmol/hr	283 071	283 071	108 773
H ₂	kmol/hr	443 682	335 434	299 474
O ₂	kmol/hr	0,674909	1,50E-16	0
S	kmol/hr	0,0046488	0,0046488	0,00113984
Mole Fractions				
CO		0,0502118	0,0377136	0,0552891
H ₂ O		0,00585525	0,152587	0,023097
CH ₄		0,00547931	0,00150229	0,000705501
CO ₂		0,00119841	0,0220497	0,000117437
N ₂		0,333846	0,359526	0,245267
H ₂		0,523265	0,426031	0,675268
O ₂		0,0795966	1,91E-17	0
S		0,000548265	0,000590438	0,000257015
Mass Flows	kg/hr	124	124	453 314
CO	kg/hr	119 255	831 733	686 819
H ₂ O	kg/hr	0,89441	216 433	184 535
CH ₄	kg/hr	0,745342	0,189757	0,050195
CO ₂	kg/hr	0,447205	764 042	0,0229213

N ₂	kg/hr	792 981	792 981	304 712
H ₂	kg/hr	89 441	676 195	603 705
O ₂	kg/hr	215 963	4,82E-15	0
S	kg/hr	0,149068	0,149068	0,03655
Mass Fractions				
CO		0,0961731	0,0670752	0,151511
H ₂ O		0,00721298	0,174543	0,040708
CH ₄		0,00601082	0,0015303	0,00110729
CO ₂		0,00360649	0,0616163	0,000505637
N ₂		0,639501	0,639501	0,672186
H ₂		0,0721298	0,0545319	0,133176
O ₂		0,174163	3,88E-17	0
S		0,00120216	0,00120216	0,000806284
Volume Flow	l/min	6460,14	10617,5	5980,53
Vapor Phase				
Molar Enthalpy	cal/mol	-663 467	-6802,05	2029,01
Mass Enthalpy	cal/gm	-453 678	-431 901	198 504
Molar Entropy	cal/mol-K	748 836	104 669	110 846
Mass Entropy	cal/gm-K	0,512054	0,664602	108 443
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Average MW		146 242	157 491	102 215
Mole Flows	kmol/hr	847 911	787 347	44 349
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H ₂ O	kmol/hr	0,0496473	120 139	0,102433
CH ₄	kmol/hr	0,0464597	0,0118282	0,00312883
CO ₂	kmol/hr	0,0101615	0,173607	0,000520822
N ₂	kmol/hr	283 071	283 071	108 773
H ₂	kmol/hr	443 682	335 434	299 474
O ₂	kmol/hr	0,674909	1,50E-16	0
S	kmol/hr	0,0046488	0,0046488	0,00113984
Mole Fractions				
CO		0,0502118	0,0377136	0,0552891
H ₂ O		0,00585525	0,152587	0,023097
CH ₄		0,00547931	0,00150229	0,000705501
CO ₂		0,00119841	0,0220497	0,000117437
N ₂		0,333846	0,359526	0,245267
H ₂		0,523265	0,426031	0,675268
O ₂		0,0795966	1,91E-17	0
S		0,000548265	0,000590438	0,000257015
Mass Flows	kg/hr	124	124	453 314
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H ₂ O	kg/hr	0,89441	216 433	184 535

CH ₄	kg/hr	0,745342	0,189757	0,050195
CO ₂	kg/hr	0,447205	764 042	0,0229213
N ₂	kg/hr	792 981	792 981	304 712
H ₂	kg/hr	89 441	676 195	603 705
O ₂	kg/hr	215 963	4,82E-15	0
S	kg/hr	0,149068	0,149068	0,03655
Mass Fractions				
CO		0,0961731	0,0670752	0,151511
H ₂ O		0,00721298	0,174543	0,040708
CH ₄		0,00601082	0,0015303	0,00110729
CO ₂		0,00360649	0,0616163	0,000505637
N ₂		0,639501	0,639501	0,672186
H ₂		0,0721298	0,0545319	0,133176
O ₂		0,174163	3,88E-17	0
S		0,00120216	0,00120216	0,000806284

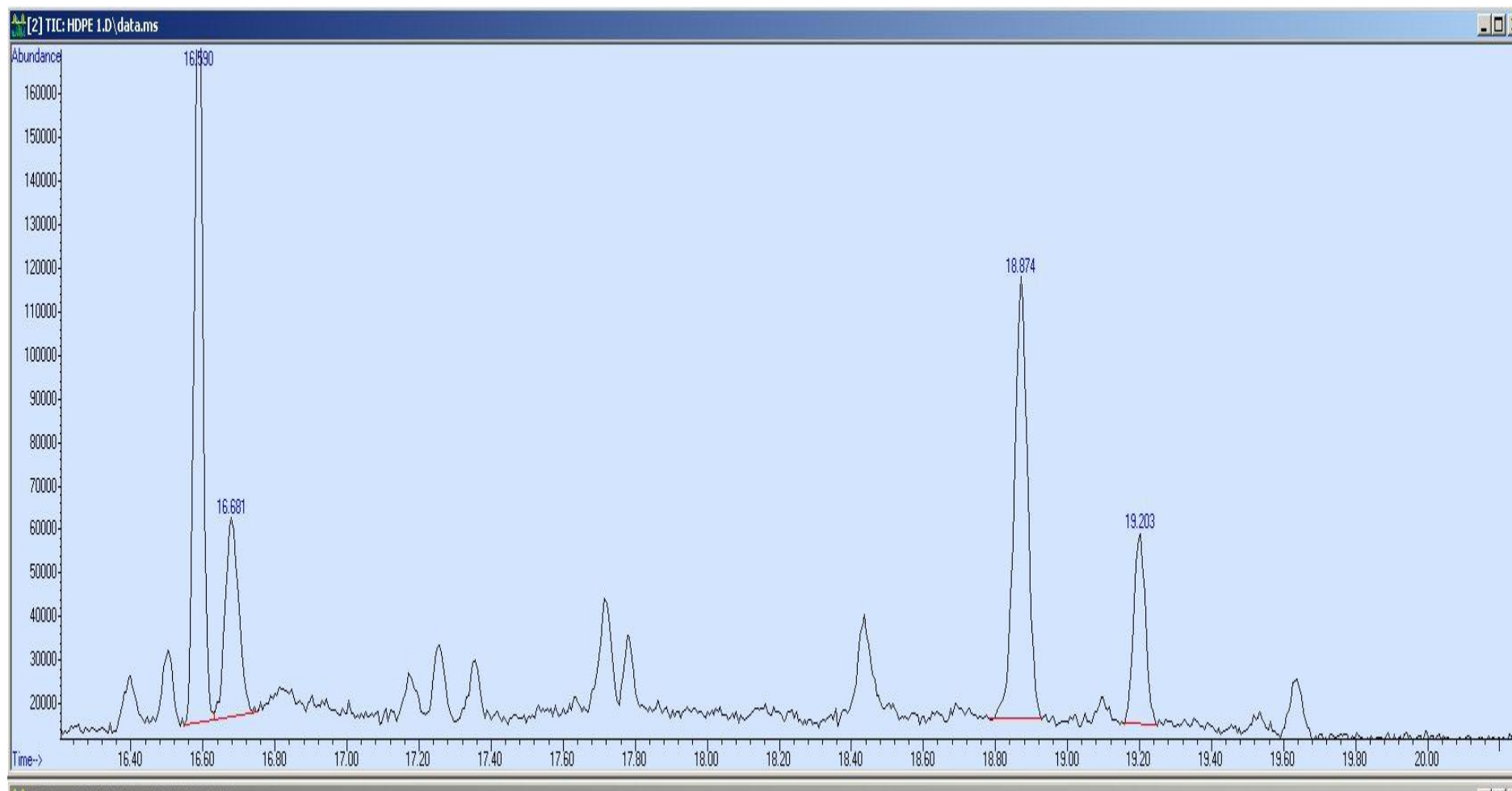


Figure 8-9: GC detailed analysis

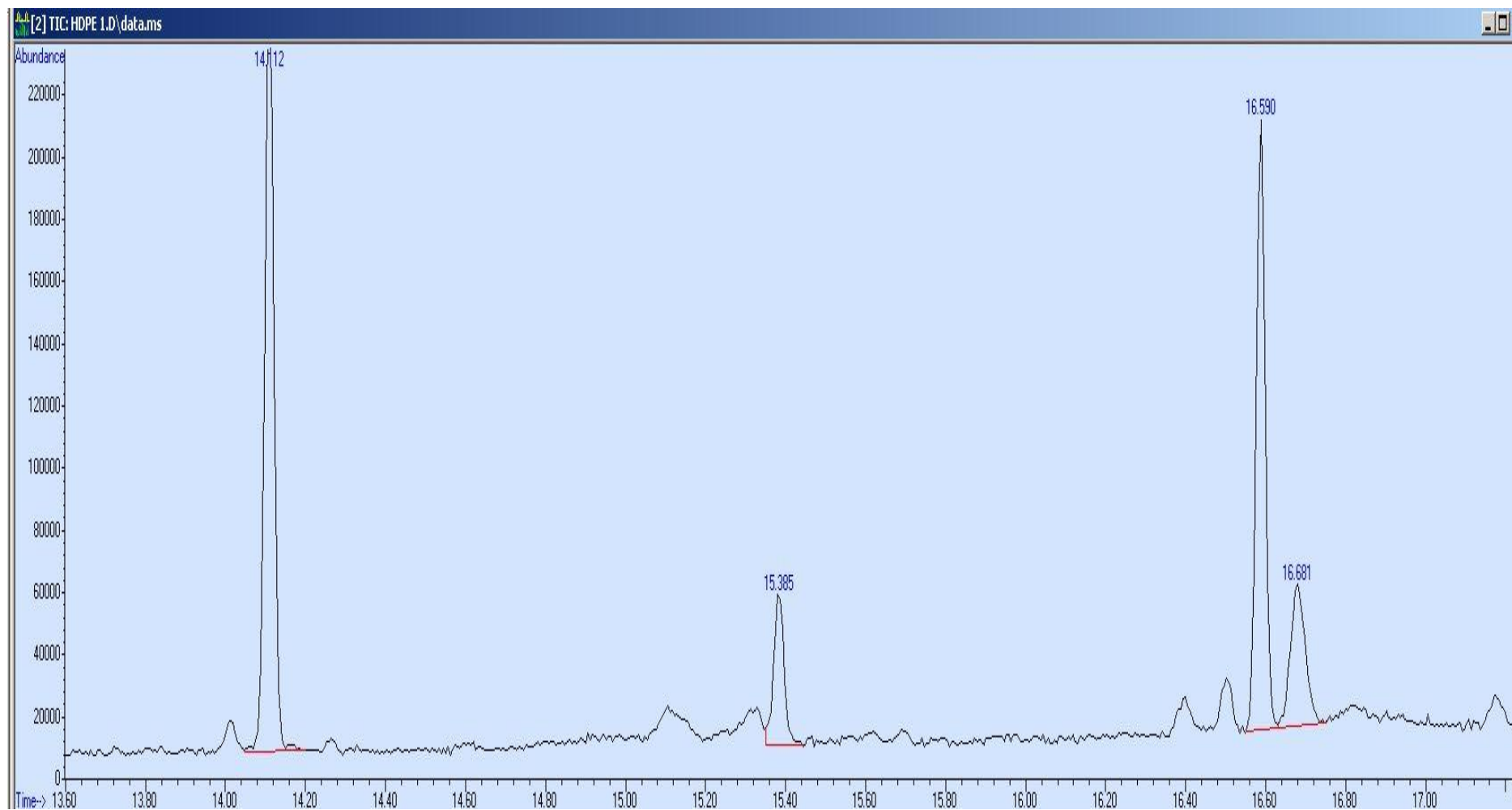


Figure 8-10: GC detailed analysis

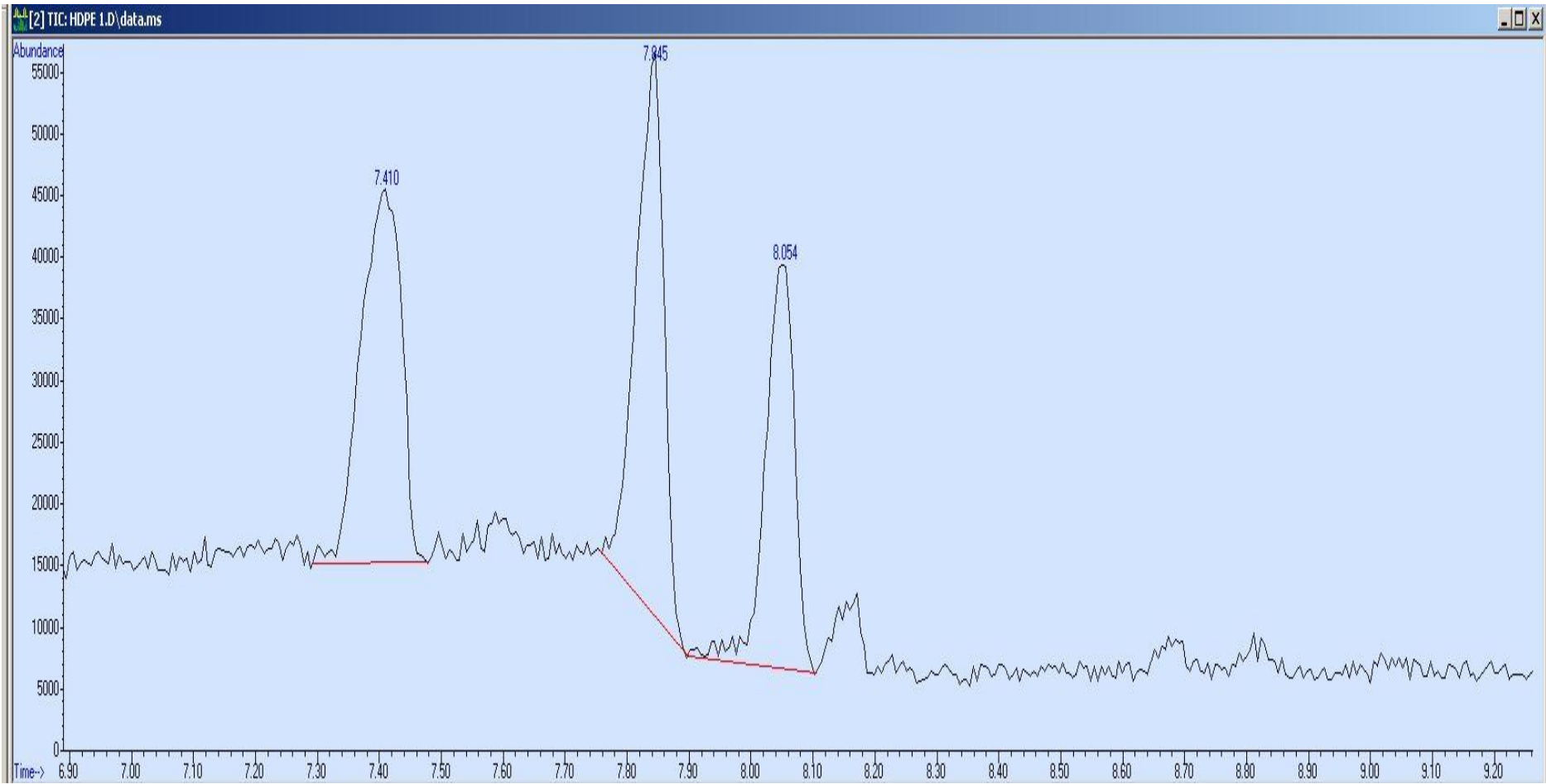


Figure 8-11: GC detailed Analysis

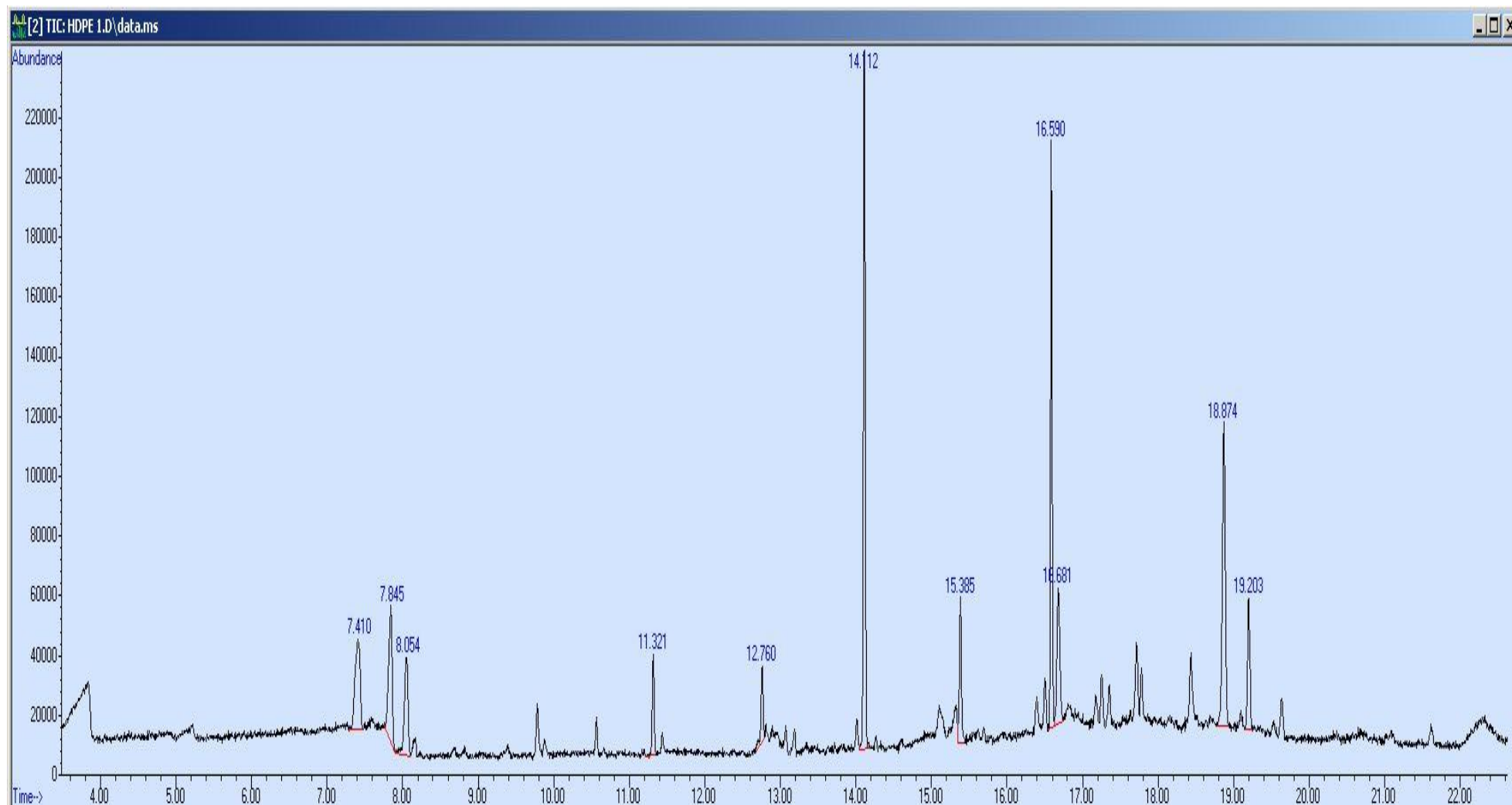


Figure 8-12: GC General Analysis

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