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Gasification of Lafia-Obi Coal Using ANSYS Fluent As CAD Tool and Effect of Temperature and Pressure on Producer Gas Composition

G. E. Ede, [1] C. O. Folayan, [2] G.Y. Pam, [3] F.O. Anafi, [4]
1 Department of Mechanical/Production Engineering Abubakar Tafawa Balewa University Bauchi Nigeria
2, 3&4 Department of Mechanical Engineering Ahmadu Bello University Zaria Nigeria
Corresponding Author: G. E. Ede

Abstract: *Gasification, the thermo-chemical conversion of fuels to combustible gases has assumed prominence because of its many advantages which include greenhouse gas sequestration, controllability among others. In this paper, Lafia-Obi bituminous coal in the Nigerian middle belt region was gasified in an updraft gasifier of 60Kw capacity. A numerical modeling and simulation of the gasification chamber was carried out using ANSYS R17.2. The model was made using solid works CAD software and then imported to ANSYS Fluent for simulation. Results obtained from the simulation showed producer gas composition of 16% CO, 15% H_2, 2.7% CH_4 and 18.6% CO_2. This is in agreement with standard range of producer gas composition. Temperatures between 299.8K (26 ^oC) to 1187K (914^oC) and pressure between 0.1 to 0.53Pa prevailed in the gasifier. As the temperature in the gasification chamber increased due to combustion reactions, mass fraction of product gas components such as carbon monoxide, carbon dioxide and hydrogen increased whereas that of methane reduced as the temperature increased. Also the mass fraction of carbon monoxide, carbon dioxide and hydrogen reduced as the pressure is increased while that of methane increased as pressure within the gasifier is increased.*

Keywords-*Coal, Gasification Chamber, Mass Fraction, Producer Gas, Simulation.*

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I. Introduction

Gasification is the thermo-chemical conversion of fuels such as coal and other biomass to combustible product gas. From the energy crises of the 1970's to date gasification has been of interest as a means of converting raw fuels such as coal and other biomass to conveniently usable forms [1]. Gasification processes have become imperative because it produces combustible gases which are used for generation of heat, power, chemicals and liquid fuels. The gas can also be used to replace natural gas which is why gasification has gained a lot of fame. Gasification also gives the advantage of controllability which is important when converting difficult fuels like sunflower and chicken dung. Emission control is another advantage of gasification as direct combustion of coal emits greenhouse gases that are responsible for acid rains.

The discovery of coal in Nigeria in 1909 [2] and consequent commencement of production in 1916 from open cast mines at Obwetti in Enugu, south east Nigeriaopened up activities in the coal industry. Subsequent prospecting was conducted and twenty-two coal mine sites/deposits were discovered with varying reserves. Lafia/Obi coal is one of them with proven reserve of 21.42 million tonnes [3]. Lafia/Obi coal is bituminous and this grade of coal is important as fuel because it burns slowly, provides a lot of heat and is gasifiable [4].

Arthur [5] analyzed the operability and optimization of an updraft gasifier using wood chips as feedstock and came up with the following: Gasification experiments were carried out at 70 l/min and 80 l/min of gasification air flow. Wood chips were consumed at rates of 2.25 kg/hr and 4.5 kg/hr respectively. A steady state model was developed for the gasifier and implemented with polymath to simulate the operation of the installation. The model was used to predict the temperature profiles in the reactor as well as concentration profiles for air flow rates of 70 and 80 l/min. The measured temperature profiles of the reactor for the different air flow were taken after 50 minutes of operation. At this time, the gasifier was considered to be in pseudo steady state. The model over predicted the production of hydrogen and under predicted the production of carbon monoxide. The model also predicted that lower tar content in the producer gas is achieved by using lower air flow rates.

Mathieu and Dubuisson, [6] also investigated the impact of Equivalent Ratio(ER) on producer gas composition. It was established that the composition of the gas changes with ER. The variations of the various gas species versus ER are more or less linear. N_2 and H_2O increases with ER from 35% up to 53% and from5% up to 15% respectively. CO and H_2 decreases from 28% down to 15% and from 21% to 7% respectively. CO_2 remains almost close to zero in the range 20 – 50% ER.

The variation in the gas composition with ER is in agreement with the findings of Sharma, [7] and Van den Eden and Silva Lora, [8] that the efficiency increases with ER until it reaches its peak at 26% ER and starts to decrease. This is basically because of the changes in gas composition as the efficiency is dependent on the volume and composition of the gas.

Williams and Larson, [9] undertook a study to establish the impact of fuel properties on gasification. They used Wyodak coal and cellulose to conduct the study. A Pyrolysis experiment was conducted. Nearly complete de-volatilisation of cellulose was found to occur below 500°C. Only about 40% of coal was de-volatilised and only after heating to close to 900°C. The slower weight loss with coal reflects its inherently lower thermochemical reactivity and much higher fraction of weight remaining even after heating to 900°C reflects the much lower content of volatile components in coals compared to cellulose.

Kuhe, [10] investigated experimentally biomass gasification in a closed top throatless downdraft gasifier using coconut shells as fuel. The fuel properties of coconut shells and its gasification feasibility were investigated. The distinctive feature of the gasifier is that it can operate successfully on coconut shell with producer gas lower heating value of 5.95mJ/m^3 and negligible clinker formation. The gasifier performed best at an equivalent ratio of 0.332 and was determined at an air flow rate of 0.00092m^3/s and coconut shell consumption rate of 0.000557kg/s. From the results obtained, coconut shells were successfully used as feedstock in the gasifier which can be used as a clean fuel for rural communities in Nigeria.

Littlewood, [11]; vanHeek and Mühlen, [12] investigated coal gasification reactions and concluded that it encompasses a series of reaction steps that convert coal containing carbon, hydrogen, and oxygen, as well as impurities such as nitrogen and sulphur into synthesis gas and other forms of hydrocarbons. This is accomplished by introducing a gasifying agent, which can be oxygen, carbon dioxide, steam, air, and/or a mixture of two or more, or all of the above into a reactor vessel containing coal feedstock where the temperature, pressure and flow pattern are controlled.

Zamzy et al., [13] designed and developed a laboratory scale updraft gasifier for gasification of oil palm fronts. The average heating value of gas was found to be in the range of 22.6% -23.36% of CO, 6.48%-68.04% H_2, 1.2%- 1.5% CH_4, 9.51%-9.65% $CO_{2,}$ with an average heating value in the range of 4.1- 4.4MJ/kg. Dry gas yield of 2.29-2.36 Nm^3/kg. Carbon conversion efficiency of 95% - 97%. Cold gas efficiency of 57%-59% and specific gasification rate of 103-109 kg/m^2h.

Chan et al., [14] conducted a Computational modeling and simulation on Korean IGCC test-bed coal gasifier to optimized burner design by CFD method. The CFD modeling was made by combining Reynolds-stress averaged Navier-Stokes equation solvers, turbulence, discrete phase and gasification reaction models. The CFD simulation method calculated the gas flow path, coal particle track, temperature, CO and H2 distributions inside the gasifier with changing the secondary oxidizer injection ratio as a burner design condition, and their calculation results are compared and examined to optimize burner design.

Wu and Chein, [15] modeled biomass gasifier with preheated air at high temperature. Effects of reaction temperature, moisture content, and preheated air temperature on biomass gasification performance such as syngas composition, cold gas and second law efficiencies, and caloric value, were studied based on a thermodynamic equilibrium model. The results indicated that the contents of the combustible species (H_2, CO, and CH_4) in the product syngas control the gasification performance. Low amounts of combustible species were reported for the conditions of high reaction temperature, high moisture content, and low preheated air temperature. Using H_2 content as a reference, there appears an optimum reaction temperature. With biomass moisture content exceeding a certain amount, reduction in combustible species was found. Although the gasification performance can be enhanced by using preheated air.

Ramzan et al., [16] studied the process of using large variety of feedstock and designs through modeling and simulation at manageable costs. Their work included the development of Steady state simulation model for gasification using Aspen Plus with particular emphasis on the influence of process operating conditions on synthesis gas composition, heating value and cold gas efficiency with various fuels. A Hybrid gasifier was modeled in three stages. The simulation results were compared with the experimental results obtained through hybrid gasifier. The performance of the simulated gasifier was compared using experimental data for Coal and Auto Shredder Waste (Used Tyres). In the simulation study, the operating parameters like Temperature, Equivalence Ratio (ER), Feed Moisture Content and Steam/Feed Injection Ratio were varied over wide range as 400-1400°C, 0.1-0.9, 5-40%, and 0.05-0.4 respectively to investigate their effect on syngas composition, High Heating Value (HHV) and Cold Gas Efficiency (CGE). It was observed that Auto Shredder Waste has maximum value of CGE (34%) at an ER of 0.28. Coal showed highest value of CGE 55% at an ER of 0.31. Among all feed stocks considered coal showed best gasification characteristics regarding Cold Gas Efficiency. Temperature increased the production of CO and H_2. Increasing ER decreased the production of CO and H_2 which decreases the CGE. Feed moisture content is an important parameter affecting the heating value of the gas. Steam injection favors hydrogen production.

Zubstov, [17] conducted an experiment with air pre-heated to 1000°C when gasifying skyline coal. The resulting producer gas was found to have a heating value of about 1400kcal/m³ (5857.6kJ/m^3). Without the pre-heated air, only 850kcal/m³ (3556.4kJ/m^3) could be achieved. When ambient temperature air was used, the resulting low combustion temperature would prevent the reactions from reaching completion resulting in low heating value gases and low conversion efficiency. It was concluded that gasification temperature does not only affects the product yield but also governs the process energy input. High gasification temperatures produce a gas mixture rich in H_2 and CO with small amounts of CH_4 and higher hydrocarbons.

Madhukar, [18] conducted simulations to investigate the impact of ER on equilibrium composition for operating conditions of Temperature. It was established that higher ER results in reduced CO and H_2 yield while that of CO_2 increases. This according to the author is due to the oxidation of H_2 and CO to H_2O and CO_2. He found out that at low values of ER, small amounts of solid carbon Cs and CH_4 are formed in the gasifier, both of which get oxidized as more air is supplied. Higher gasification efficiencies are achieved at lower ER for fuel with higher moisture content. Gasification efficiency decreases at higher equivalence ratios.

Altafini et al., [19] carried out simulations to establish the impact of pressure on gas composition. It was reported that the increase in pressure results in reduced hydrogen and Carbon monoxide volumes. It was also established that very low pressures (10.13kPa) result in an increase in the yield of H_2.

Baker, [20] wrote on the components and operations of fixed bed gasifier. He looked at the factors influencing the efficiency of fixed bed biomass gasifier systems. In the reactor, biomass is heated by combustion. Four chemical processes were distinguished, namely drying, pyrolysis/carbonization, oxidation (combustion) and reduction reactions. Combustion occurs in the oxidation zone.

Onwu, [21] explored new technologies on coal power plants. He reiterated that a modern coal power plant could be a modification of existing designs with emphasis on unit operations such as the combustion system, the heat extraction, combined cycles and clean coal aimed at minimizing the pollution level. The author concluded by saying that electricity generation through coal-firing plants is a good option for the coal producing areas of Nigeria.

Several other research works on Nigerian coals and their metallurgical and power generation potentials have been carried out. However, none of them to the best of our knowledge have worked on the gasification of Lafia-Obi coal and the numerical modeling and simulation of the gasification chamber.

This paper therefore covers the gasification of Lafia-Obi coal and the characterization of the producer gas. It also includes a numerical modeling and simulation of the gasification chamber. Results were compared with standard producer gas composition of gasification with coal and other biomass resources.

II. Methodology

The updraft gasifier system consists of a screw conveyor embedded in a feedstock hopper, the gasification chamber or reactor, a cyclone, a wet scrubber and a gas filter. A centrifugal blower with a regulator delivers a measured amount of air(62l/min from design calculation) to the gasification chamber. In the gasifier 25kg (as per design calculation) of bituminous coal is broken down by the use of heat in an oxygen-deficient environment to yield a combustible product gas. The isometric view and assembly drawing of the gasification system is shown in figures 2.1 and 2.2.The heat for gasification is generated through combustion of part of the coal feed material on the grate of the reactor.

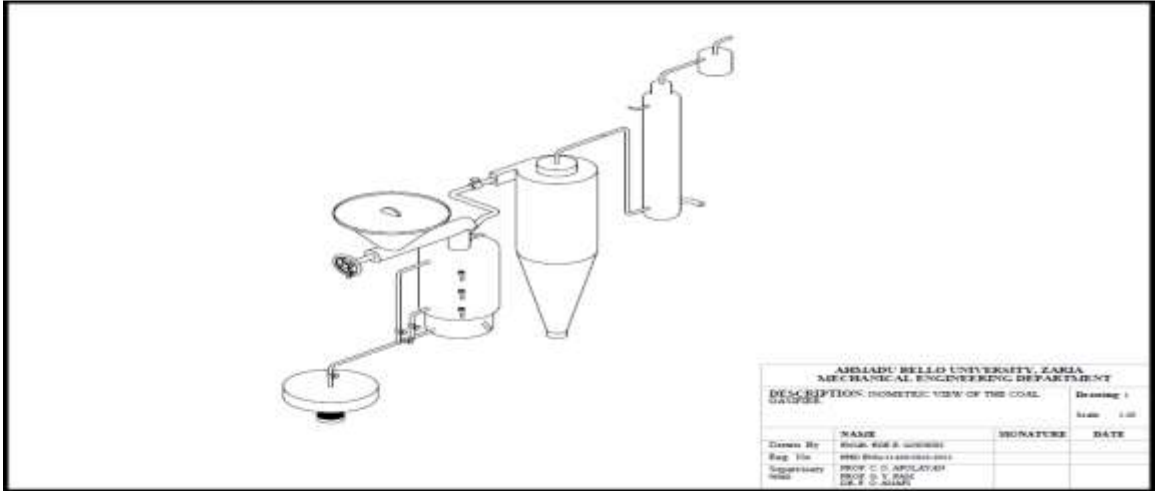

Figure.2.1. Isometric view of the coal gasification system

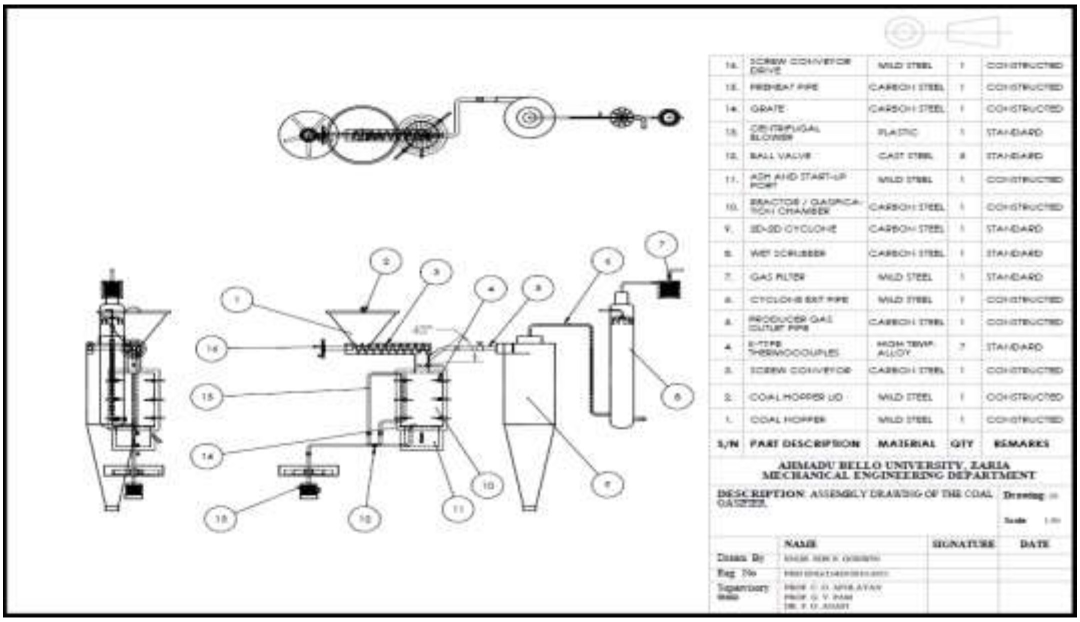

Figure.2.2. Assembly drawing of the coal gasification system

When coal is gasified under practical conditions, the following reactions take place [22];

$$\text{Coal} \xrightarrow{\text{PYROLYSIS}} \text{Char(C)} + \text{Coal Volatiles (VM)} \qquad (1)$$

Where VM is volatile matter. Volatile Matter includes all gases, tars and light hydrocarbons. Reactions with -ΔH are endothermic while those with +ΔH are exothermic.

$$VM + H_2 \xrightarrow{\text{HYROCRACKING}} CH_4 \;\; +\Delta H \qquad (2)$$

$$VM + H_2O \xrightarrow{\text{GASIFICATION}} CO + H_2 \;\; -\Delta H \qquad (3)$$

$$C + 2H_2 \xrightarrow{\text{HYDROGASIFICATION}} CH_4 \;\; +\Delta H \qquad (4)$$

$$C + H_2O \xrightarrow{\text{GASIFICATION}} CO + H_2 \;\; -\Delta H \qquad (5)$$

$$C + CO_2 \xrightarrow{\text{GASIFICATION}} 2CO \;\; -\Delta H \qquad (6)$$

$$CO + H_2O \xrightarrow{\text{SHIFT CONVERSION}} CO_2 + H_2 \;\; -\Delta H \qquad (7)$$

$$C + O_2 \xrightarrow{\text{COMBUSTION}} CO_2 \;\; +\Delta H \qquad (8)$$

The updraft coal gasifier was designed using relevant design equations and criteria. The model equations adopted from the work of Moonkyeong et al., [23] are as follows;

$$C_aH_bO_cN_dS_e + \left(\frac{a}{\phi}-\frac{b}{4}-\frac{c}{2}-\frac{e}{2}\right)O_2 \rightarrow \left(\frac{2}{\phi}-1\right)aCO_2 + 2\left(1-\frac{1}{\phi}\right)aCO + \left(\frac{b}{2}-e\right)H_20 + eH_2S + \frac{d}{2}N_2 (9)$$

$$C_aH_bO_cN_dS_e + aCO_2 \rightarrow 2aCO + cH_2O + \left(\frac{b}{2}-c-e\right)H_2 + eH_2S + \frac{d}{2}N_2 (10)$$

$$C_aH_bO_cN_dS_e + (a-c)H_2O \rightarrow aCO + \left(a+\frac{b}{2}-c-e\right)H_2 + eH_2S + \frac{d}{2}N_2 \; (11)$$

$$C_aH_bO_cN_dS_e + \left(2a-\frac{b}{2}+c+e\right)\mathrm{H_2} \rightarrow \mathrm{aCH_4 + cH_2O + eH_2S} + \frac{\mathrm{d}}{2}\mathrm{N_2} (12)$$

$$\phi = \frac{2z+2}{z+2}\;;\ \text{wherez} = 2500\exp\left(\frac{6249}{T}\right)$$

For Lafia-Obi bituminous coal used, the coefficients a, b, c, d and e are 137, 97, 9, 1 and 1 respectively.

Coal reacts with oxygen in the air to produce CO, CO_2 and H_2O. Coal also reacts with CO_2 and steam to produce CO and H_2 in the solid phase as seen in equations 9 to 12.

$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \rightleftharpoons \mathrm{CO_2} (13)$$

$$\mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \rightleftharpoons \mathrm{H_2O} \; (14)$$

$$\mathrm{CO + H_2O \rightleftharpoons CO_2 + H_2} (15)$$

$$\mathrm{CO + 3H_2 \rightleftharpoons CH_4 + H_2O} \qquad (16)$$

The combustible gases (CO and H_2) in turn reacts with oxygen in the gaseous phase to produce more heat. Carbon monoxide is converted to hydrogen by water-gas shift reaction while methane is produced by hydrogasification of char as seen in equations 13 to 16.

The gasification chamber or reactor was modeled using solid works computer aided design (CAD) software and then imported to ANSYS Fluent using the geometric tab selection. The geometry of the gasifier was meshed by creating named selection for air inlet, fuel inlet and outlet, the symmetry surface, the outer wall boundaries were automatically detected by ANSYS Fluent. The mesh parameters were adjusted to finer mesh, relevant center changed to fine and smoothing changed to high.

The CFD simulation set up tab was selected and launched. The 3-D, display mesh after reading, embed graphics windows and workbench colour scheme options were enabled. Also enabled were the double-precision and serial processing tabs. The default settings of pressure-based steady-state solver in the solver group box were retained. The model was specified by enabling the energy equation, the standard k-epsilon turbulence model and a value of 1 entered for energy iterations (one energy iteration).

The materials and properties were defined by specifying the continuous phase material and selecting the wsggm (weighted-sum-of-grey-gases-model) domain. The CFD solution for reacting flows are sensitive to boundary conditions, for this reason appropriate boundary conditions based on design calculations were specified for inlet air, coal and outlet atmospheric pressure as follows:
Air inlet: 20bars
Air temperature: 300K -1000K
Turbulence: 10%
Hydraulic diameter (diameter of air pipe): 50mm
Mass flow: 62L/min (from design calculations)
Coal inlet parameters;
Pressure: 0
Temperature: 800K (as per standard gasification practice)
Turbulence: 10%
Hydraulic diameter: 500 mm (gasification chamber diameter; as per design calculations)
Amount of coal: 25kg/hr. (As per design calculations)
Coal component: Carbon (79.1%), Hydrogen (5.0%), Oxygen (6.4%), Nitrogen (1.7%), Sulphur (1.66%), ash (4.54%) and water (1.6) as per ultimate analysis.

The solution was obtained by selecting the couple tab. The solution controls were set up by enabling the display residuals tab and the plot tab in the option group box. The flow field was initialized by retaining the default hybrid initialization, initializing the solution saving case file and starting the calculation by requesting 1500 iterations. The solution converged at about 700 iterations and was saved.

The results were displayed by enabling "filled" option, "select temperature" option "static temperature" option, "symmetry" option and "display" option. The temperature profile was displayed. Similar procedure was followed for probing producer gas mass fraction and pressure profiles.

III. Results And Discussion

The following results were obtained for the CFD simulation carried out using ANSYS R17.2.

Figures 3.1 to 3.7 shows the results which include the mesh of the gasification chamber, carbon monoxide mass fraction, hydrogen mass fraction, methane mass fraction, carbon dioxide mass fraction, temperature profile and pressure profile respectively.

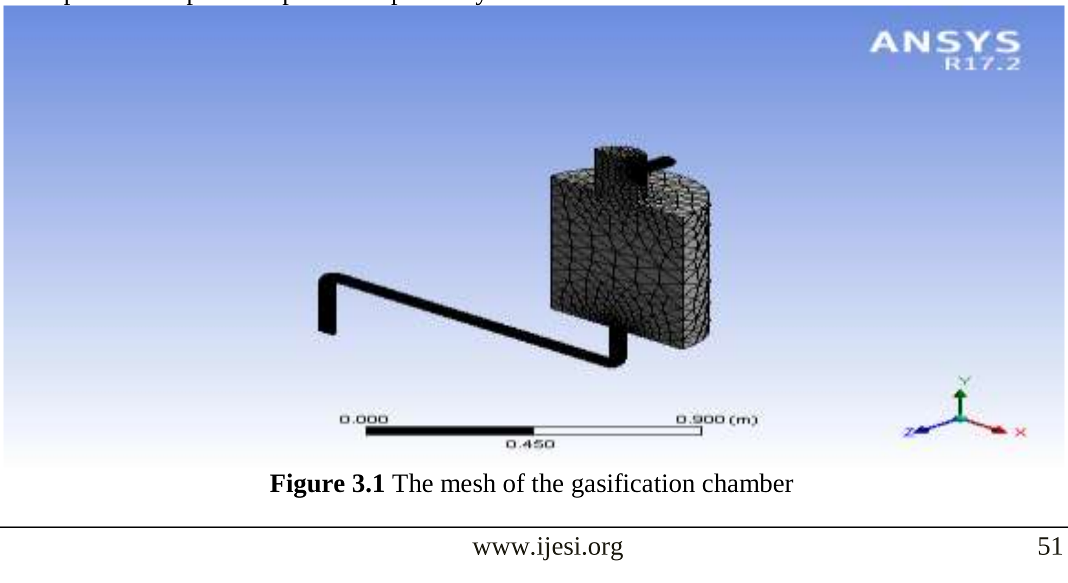

Figure 3.1 The mesh of the gasification chamber

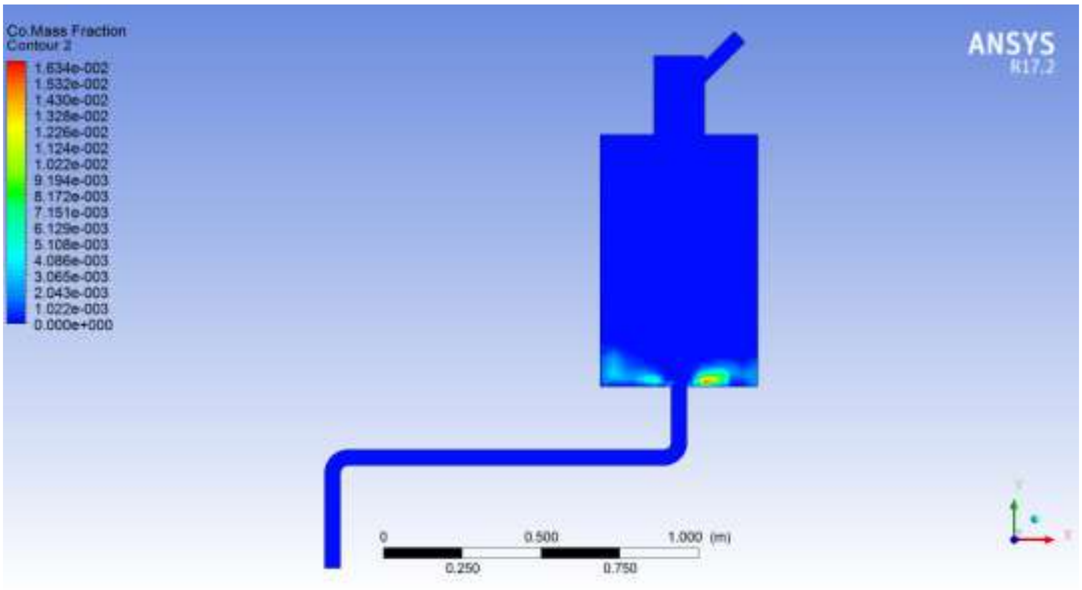

Figure 3.2 Carbon monoxide mass fraction profile

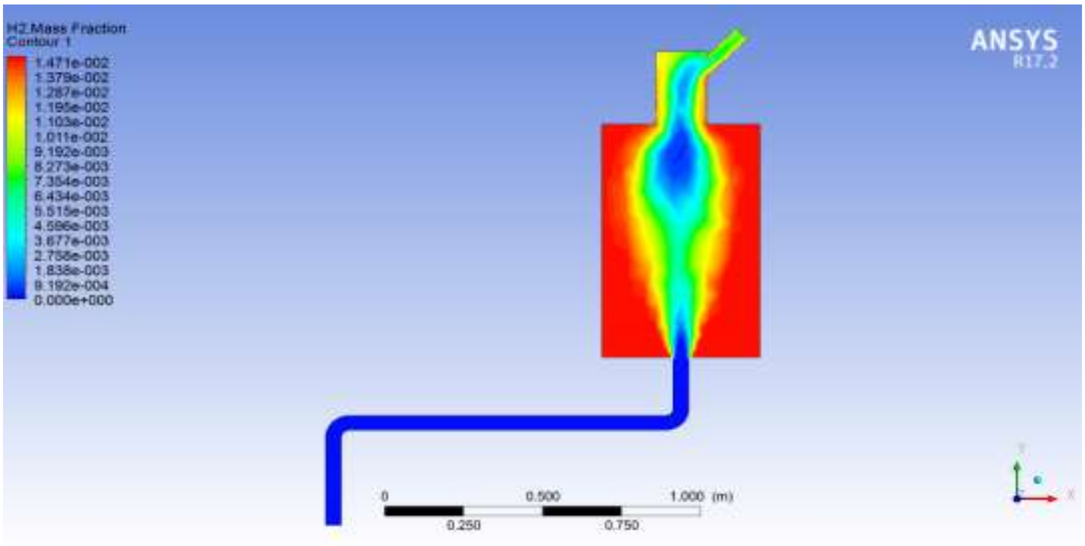

Figure 3.3 Hydrogen mass fraction profile

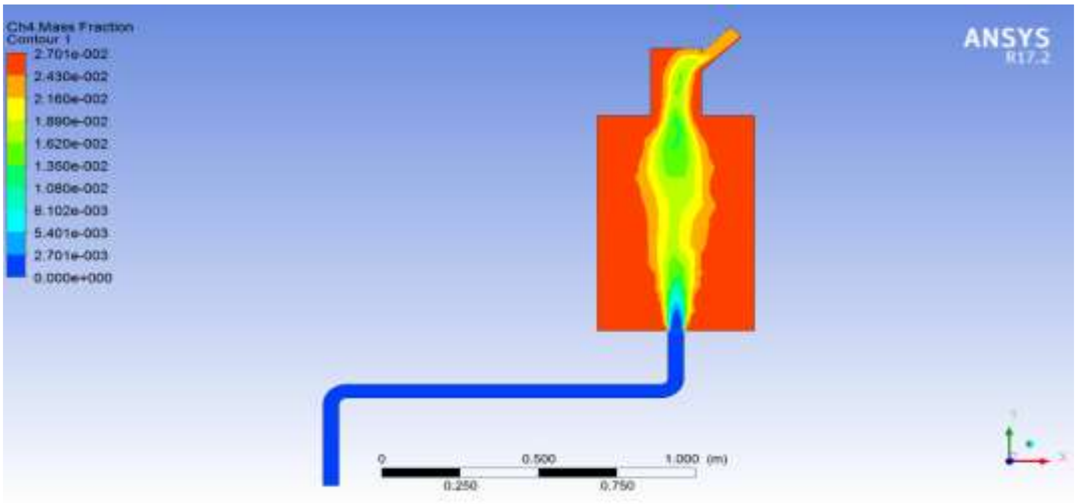

Figure 3.4 Methane mass fraction profile

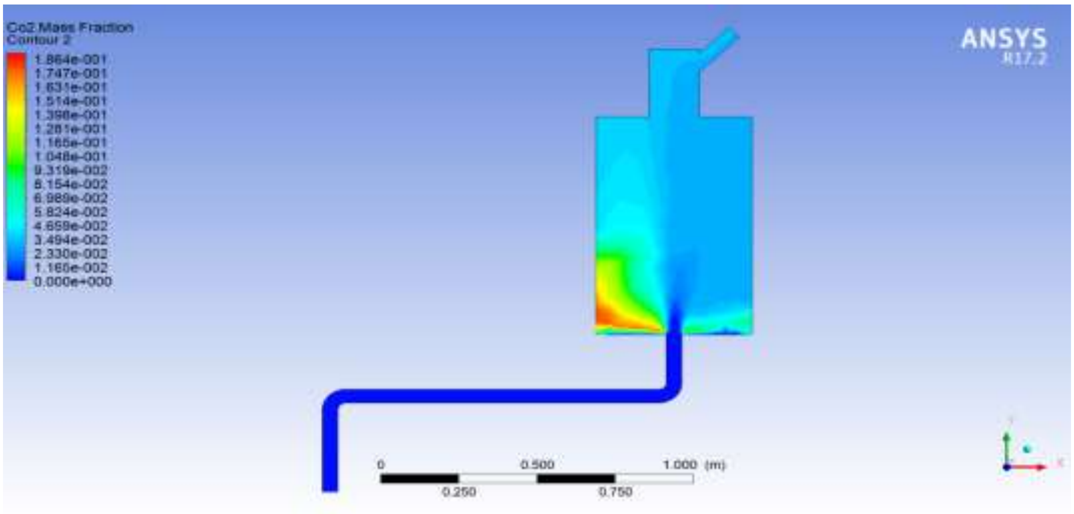

Figure 3.5 Carbon dioxide mass fraction profile

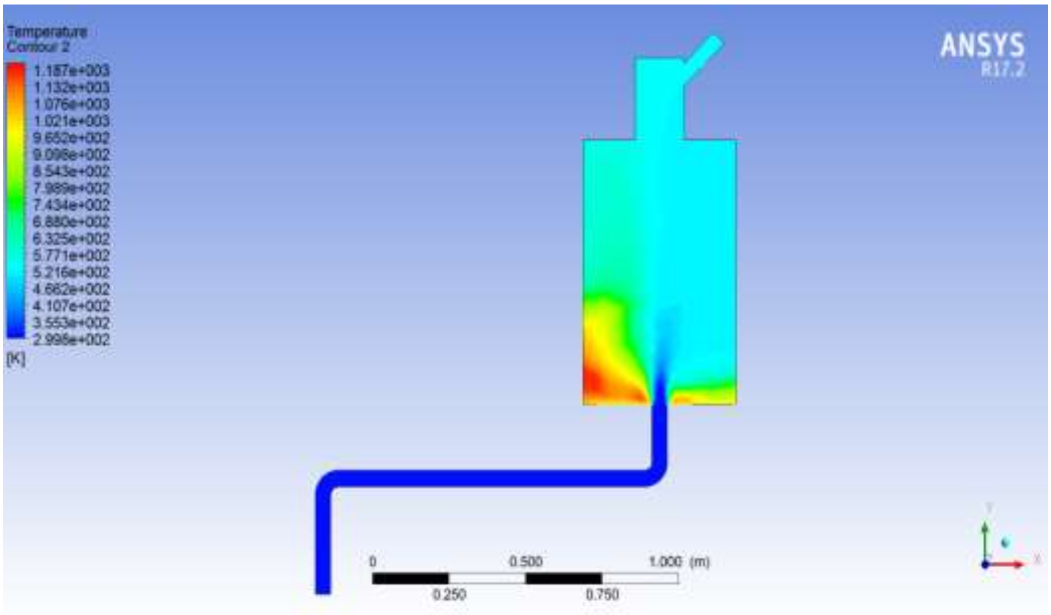

Figure 3.6 Temperature profile of the gasifier.

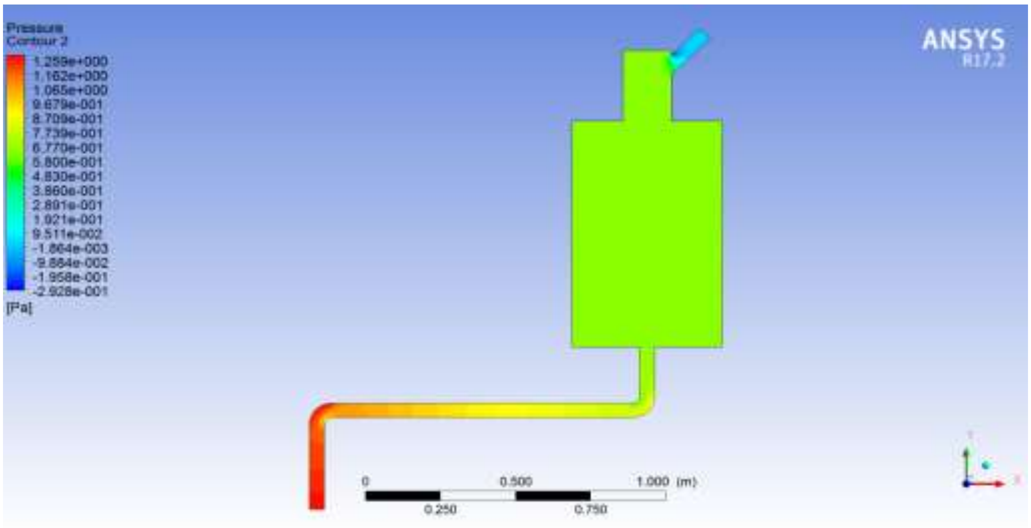

Figure 3.7.Pressure profile of the gasifier.

3.1 Effect of Temperature and Pressure on Producer Gas Composition

The gasifier temperature affects the composition of syngas. Gasification involves oxidation and reduction reactions taking place simultaneously. At very low temperature the fuel is not completely converted. When temperature increases due to combustion reactions the fuel is converted into carbon dioxide, carbon monoxide and other gases. Reduction reactions and carbon monoxide shift reaction increase the conversion of coal into carbon monoxide and hydrogen.

A graphical representation of the effect of temperature on synthesis gas composition is shown in Figures 3.8. As the temperature inside the gasifier increases, the mass fraction of carbon monoxide, carbon dioxide and hydrogen increases around the gasifier to a maximum value of 0.16 (16%), 0.186 (18.6%) and 0.15 (15%) respectively whereas that of methane reduces as the temperature increases from 0.027 (2.7%) until it becomes zero at the hearth region where the temperature is very high.

The reason for this is that the reactions producing CO, CO_2 and H_2 are endothermic and are favoured at high temperature while the reactions producing methane are exothermic and favoured at low temperature. Also at high temperature, methane formed gets combusted resulting in low methane yield.

The standard range of producergas composition according to [24] are; 9-15% CO, 17-22% CO_2, 12-20% H_2 and 2-3% CH_4. The composition of producer gas obtained in this research work is in agreement with this standard specification.

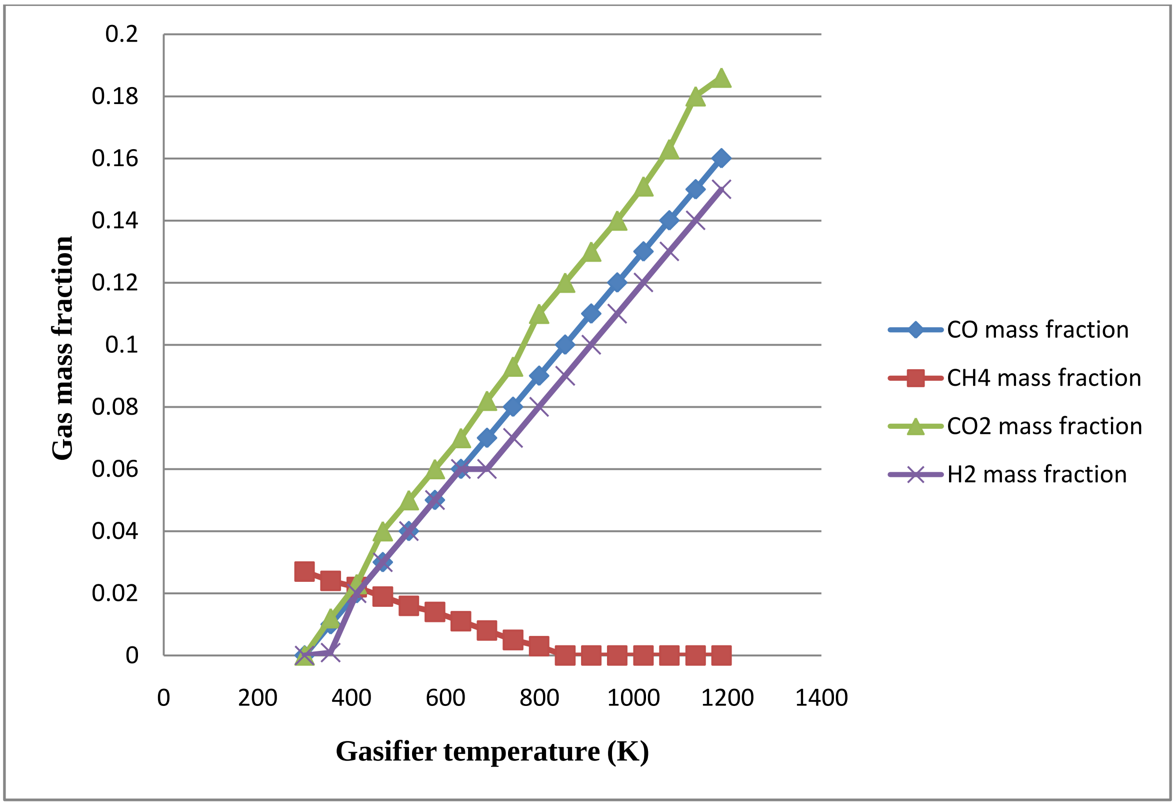

Figure 3.8 Effect of Temperature on Synthesis Gas Composition

The variation of product gas mass fraction with pressure is shown in figures 3.9. As the pressure increases along the gasifier from 0.1 to 0.53Pa, the mass fraction of methane increase whereas the yield of CO, CO_2 and H_2 decreases. Production of methane is favoured at relatively high pressure. This is because the reactions producing methane are exothermic and are favoured at high pressure while the reactions producing CO, CO_2 and H_2 are endothermic and favoured at low pressure.

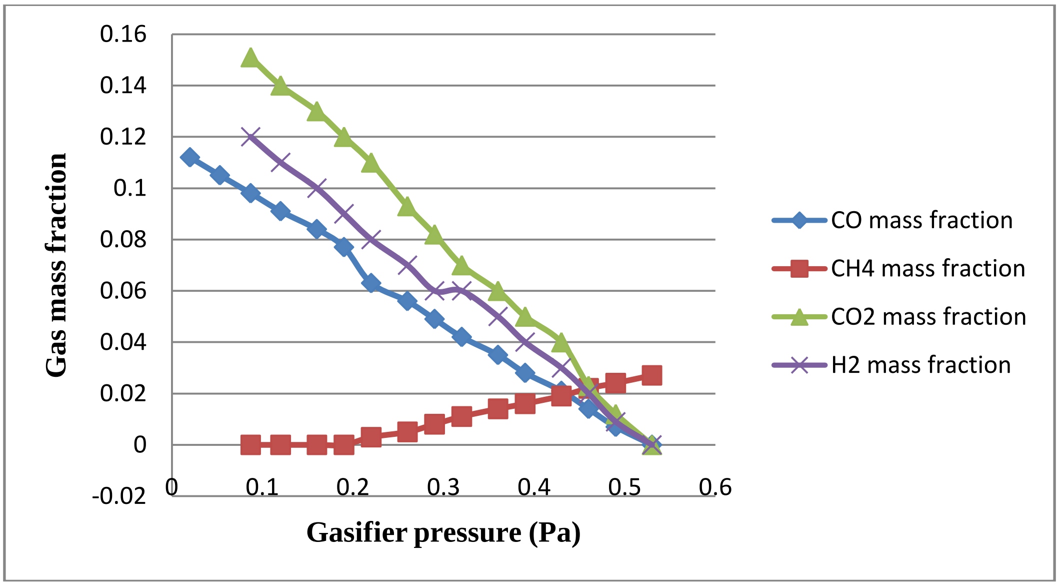

Figure 3.9 Effect of pressure on synthesis gas composition

IV. Conclusions

On the basis of results obtained from this research work, the following conclusions can be drawn:

1. As the gasifier temperature increased, the yield of carbon monoxide, carbon dioxide, and hydrogen increased while that of methane decreased.
2. As the pressure within the gasifier increased, the yield of carbon monoxide, carbon dioxide and hydrogen decreased while that of methane increased.
3. The results obtained from this work are in agreement with standard gasification results.

These conclusions are important for controllability (setting the conditions for obtaining desired products) and their amounts.

An experimental validation of results obtain in this work is ongoing and results will be published accordingly.

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