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# Investigating the Suitability of Morupule Coal for Coal Gasification Technology

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*ABSTRACT*

*The widespread occurrence and availability of coal makes it the world's prime source of energy for different end use applications. Coal is commonly used for electricity production through coal combustion. However, many researchers have indicated that coal combustion is a prime contributor to emission of greenhouse gases contributing to global warming. During combustion gaseous elements such as sulfur, hydrogen, carbon and nitrogen react with oxygen to produce their respective oxides. These oxides contribute to global warming, air and water pollution as well as acid deposition. Emission of these oxides and their effect on the environment has resulted in increased interest in clean coal technologies. Clean coal technologies, such as coal gasification technology, use multiple technologies to control the emissions so as to minimize environmental effects from coal utilization.*

*In this paper, the characteristics of Morupule coal from the south and east main sections are determined to establish its suitability for gasification. The characterization was conducted using thermal analysis (Thermogravimetric Analyzer) and an X-Ray Fluorescence (XRF). Numerical simulation was also carried out using Ansys software for species transport. The samples proved the coal to be from a high ash and sulfur content and medium volatiles bituminous parent rock, whilst species transport revealed a sufficient syngas yield per kilogram of coal for downstream processes.*

## INTRODUCTION

Coal still remains the centre of the global energy system by accounting for approximately 40% of the world's electricity production. Due to its abundance, wide distribution and affordability, coal is also expected to take the position of petroleum as the world's prime source of energy in a few years[1]. During power generation, coal is burnt to produce steam that drive turbines. However, coal combustion is a major contributor to the emission of greenhouse gases and other pollutants. Its chemical structure is made up of elements like sulphur, carbon and nitrogen that when released react with oxygen to form sulphur dioxide ($SO_2$), carbon dioxide ($CO_2$) and nitrogen oxides ($NO_x$) Due to this, comprehensive data on coal properties is required in-order to estimate the performance of the coal during conversion processes like combustion, gasification or liquefaction[2;3;4]. Such data is also essential in assessment and utilization of coal for evaluation of environmental impact and developing geological and geochemical models to assist in interpretation and prediction of coal quality[3].

Coal also consists of mineral matter in the form of mineral phases and inorganics such as silicates, sulphides and carbonates[5]. A review on analysis, origin and significance of mineral matter in coal was done by Ward [6]. Ward [6]outlined the methods that can be used in evaluating the mineral content in coal, and their modes of occurrence.

Mohammad et.al.[7] investigated the characterization of bituminous and sub-bituminous coals together with their bottom ashes from a coal-fired power plant in-order to determine their moisture content, loss of ignition and heat of combustion. It was reported that the level of ignition (LOI) is directly proportional to the carbon content in coal.

Gupta [2] carried out a review of advanced characterization of coal and concluded that coal being heterogeneous in nature needs different analytical techniques to accurately predict its performance during combustion, gasification or liquefaction processes. Analysis for ash, fusion temperatures and proximate properties were performed for the bulk properties (assuming coal to be a homogeneous material). Advanced bulk analytical techniques provided data on organic structure of coal while chemical fraction method provided data on inorganic matter. The techniques and modelling procedures were discussed to better understand the behaviour of coal during chemical conversion.

Several studies have been done on coal properties relating mainly to emissions of particulate matter, sulfur, trace elements and green-house gases due to great emphasis placed by the international climate acts such as the Clean Air Act Amendment ( US Statutes at Large, 1990, Public Law 101- 549)[8] on the energy industry. In-order to comply with these international climate regulations, the study was done to determine properties of Morupule coal for the calculations of emissions, heating value and efficiency. It also established the flow of gaseous fuels in the reactor as a way of determining its viability for coal gasification technology.

## MATERIALS AND METHODS

### Materials

Coal samples used for the analysis were from the East Main and South sections of the main seam that is currently being mined at Morupule Colliery in Palapye. The samples were only washed with water to reduce dirt and there was no chemical treatment. They were then air dried. The particle size used was 2.5mm.

### Methods

#### *Determination of proximate and ultimate properties*

Proximate analysis was carried-out in a thermogravimetric analyser (TGA 701). It was based on monitoring changes in weight sample as they were progressively heated under different conditions. The following equations were used for calculating the proximate properties of coal[9];

$$Moisture = \frac{Initial\ mass - Moisture\ mass}{Initial\ mass} * 100\% \tag{1}$$

$$Volatile = \frac{Moisture\ mass - Volatile\ mass}{Initial\ mass} * 100\% \tag{2}$$

$$Ash = \frac{Ash\ mass}{Initial\ mass} * 100\% \tag{3}$$

$$Fixed\ carbon = 100 - (Moisture + Volatile + Ash) \tag{4}$$

Where moisture, volatile mass and ash mass are lost mass at end of moisture step, volatile step and ash step respectively.

The elemental composition of the coal was determined through ultimate analysis (5E-CHN2200 Ultimate analyser) experiments that were carried out by Morupule Colliery in accordance with the ASTM D5373 standard.

### *Combustion analysis*

Combustion analysis is generally done in-order to improve the fuel economy, reduce exhaust emissions as well as to improve the safety of equipment used for combustion[10]. Analysis for combustion behaviour in this study included determining the total amount of air required during combustion, total volume of flue gases emitted, maximum $CO_2$ and $SO_2$ emitted, and ash analysis. Since the analysis was done by use of theoretical equations from the literature [10, 11], a comparison was made between direct combustion and gasification processes in-order to determine the improvement when utilising the coal in gasification process. The following equations were used for calculations in combustion analysis;

Total amount of air required for combustion

$$kg\ of\ air\ per\ kg\ of\ fuel = 11.53C + 34.34\left(H_2 - \frac{O_2}{8}\right) + 4.29S \tag{5}$$

Where C, H, S and O are carbon, hydrogen, sulphur and oxygen respectively.

Total amount of air required during gasification

$$stoichiometric\ air = \%C * \frac{23}{12} + \%H_2 * \frac{23}{4} + \%S * \frac{23}{32} \tag{6}$$

Total volume of flue gases emitted during combustion

$$V_s = 1.85C + 11.11H + 0.68S + 0.8N + 1.24W \tag{7}$$

Total volume of flue gases emitted during gasification

$$V_s = \%C * \frac{23}{12} + \%H_2 * \frac{23}{12}\%S * \frac{23}{32} + stoichiometric\ air * 0.79 \tag{8}$$

Where $W$ is coal moisture content

Maximum $CO_2$ and $SO_2$ emissions during combustion

Maximum $CO_2$ from carbon content

$$maximum\ \%CO_2 = \frac{CO_2 moles}{CO_2 moles * N_2 moles} * 100\% \tag{9}$$

$$maximum\ \%CO_2\ by\ volume = maximum\ \%CO_2 * \frac{21-\%O_2 measured}{21} \tag{10}$$

Maximum $SO_2$ from sulphur content

$$maximum\ \%SO_2 = 0.95 * \%S \tag{11}$$

Maximum $SO_2$ from gasification reaction equation

$$maximum\ \%SO_2 * \frac{23}{32} \tag{12}$$

### *Ash analysis*

An X-Ray Fluorescence technique was used to determine the major and minor constituent elements contained in ash from the coal samples. The detected elements were then used in calculating deposits of unfavourable residues in the furnace by determining the rate of fouling and slagging caused by ash. The following equations were used to calculate the rate of fouling and slagging [10 ;11;12];

Alkalinity/acidity index (base/acid ratio)

$$\frac{B}{A} = \frac{\%(Fe_2O_3+CaO+MgO+Na_2O+K_2)}{\%(SiO_2+Al_2O_3+TiO_3)} \tag{13}$$

Slagging Index (Rs)

$$Rs = \frac{B}{A} * St^d \tag{14}$$

Fouling Index (Rf)

$$R_f = \frac{B}{A} * (Na_2O + K_2) \tag{15}$$

Alkali Index, AK

$$AK = Na_2 + 0.96559 K_2O(\frac{A^d}{100}) \tag{16}$$

The alkalinity level is used to determine the possibility of mineral deposits on furnace surfaces and also for predicting absorption levels of sulphur dioxide in ash. It has been noted that the absorption levels of sulphur dioxide in ash does not exceed 15% of the total sulphur produced[14].

$$sulfur\ absorption = 0.15 * SO_2 produced \qquad (17)$$

### *Calorific value*

The amount of energy contained in coal sample was determined using a high volume bomb calorimeter – AC600.

### *Numerical Simulation of gaseous fuels*

Numerical simulation was carried out to establish the flow of gaseous fuels in the reactor during gasification. The simulation was conducted using Ansys Fluent software. The governing equations implemented were continuity, momentum and energy equations, discretized into algebraic equations to be solved numerically using the same software. A 3-D computational fluid dynamics transient state model was incorporated to solve for the transport of gaseous fuels using the Eulerian model[15]. Flow turbulence was determined by realizable k-Ɛ model and equations for transport of different species in syngas resolved with Finite rate/Eddy-dissipation model. Coal particles were regarded as a separate secondary phase and distributed in the gas phase by the discrete phase model. The simulation process was initiated at 800K, $5*10^5$ Pa, 0.5 oxygen-steam ratio and 15kg/s coal feed rate.

The following assumptions were made during the simulation process;

- Pressure at the outlet was considered similar to atmospheric pressure
- There was no slip wall condition for both phases
- Volume fraction at the inlet for the solid phase was zero
- Pyrolysis process was completed at coal feed position as drying process and devolatilization reactions occurred quickly.

### *Gasification efficiency*

Gasification efficiency was calculated as the ratio of the energy content of the synthesis gas to the ratio of the energy content of coal[16].

$$\text{Gasification efficiency, GE}=\frac{HHV_S*Q_S}{HHV_C*m_C} \qquad (18)$$

Where HHV, $Q_s$ and $m_c$ are higher heating value, syngas volumetric flow rate and coal feed rate respectively.

### *Gasification yield*

The syngas yield was calculated from the volume of synthesis gas given out per unit mass of coal used in the reactor[16]. The sample mass was on dry basis.

Gasification yield, $GY=\frac{Q_s}{m_c}$ (19)

## RESULTS ANALYSIS AND DISCUSSION

### Analysis of proximate and ultimate properties

The results for proximate and ultimate properties are presented in Table 1

Table 1: Proximate and ultimate properties

| Proximate Analysis | Content (%) | Ultimate Analysis | Content (%) |
|---|---|---|---|
| Moisture | 4.9 | Carbon | 61.7 |
| Volatile matter | 24.4 | Hydrogen | 3.2 |
| Fixed carbon | 47.3 | Nitrogen | 1.4 |
| Ash | 23.4 | Sulphur | 0.8 |
|  |  | Oxygen | 8.3 |

The results for proximate and ultimate properties are in agreement with the results obtained by National Energy Strategy (NES) [16]. During their study, it was noted that coal contained moisture ranging from 5% to 70%, range for fixed carbon was 50% to 98% while volatile matter measured in the absence of ash and moisture varied from 2% to 50%. The study also revealed that coals could produce ash of up to 40%. The results for ultimate analysis carried out by NES indicated most coals with carbon content less than 90% usually have hydrogen content below 5% while all coal types have nitrogen content between 1% and 2%. The study also indicated that coals with 65% carbon content or less may contain oxygen of up to 30% and that most coals contained sulfur ranging from 0.5% to 2%. The results for sulfur content also correlated with those of Chou [17], who reported that sulfur levels in coal could reach a maximum of 1.4%. The 0.8 % is close to the 1.4% maximum, reported by Chou [17] and this indicates that the samples are from high sulfur coal.

When characterizing the coal samples, reference was made to studies carried out by Bowen et.al [18] on the formation of different types of coal. The results of the study by Bowen et.al [18] gave ranges for fixed carbon, volatile matter, calorific value, moisture, sulfur and ash content that were used for classifying different types of coal. The results from the present study had coal samples in the range of bituminous coal for fixed carbon; range of anthracite and bituminous coals for moisture content; range of lignite for ash and sulfur content. The calorific value for the samples was above all the ranges indicated by Bowen et.al. The data for proximate properties indicated that the coal samples were from a medium volatile bituminous parent rock. Classification basing on the amount of volatile matter correlated with the results achieved during the study on coal classification and origin [16, 19]. The authors [16, 19] used the volatile matter content to classify coal and noted that coal containing volatile matter between 22% and 31% falls in the rank of medium bituminous coal. It was also noted that coal with moisture content of 5% to 10% can be classified as bituminous coal. The samples under study had heating value of 23MJ/kg. The high calorific value is good in maintaining good flame stability performance at low loads without the necessity for back-up fuel support[14].

## Combustion analysis

Comparison of fundamental parameters between coal direct combustion and gasification

Table 2: Combustion analysis results

| | **Direct Combustion** | **Gasification** |
|---|---|---|
| **Air required($m^3$/kg)** | 2.5 | 1.22 |
| **Gaseous emissions** | | |
| Flue gases | 1.57 | 1.25 |
| Carbon dioxide | 0.178509 | 0.09 |
| Sulphur dioxide | 0.7125 | 0.001 |
| **Ash($m^3$/kg)** | | |
| Sulphur in ash | 0.106875 | 0.000151185 |

Table 2 makes a comparison of fundamental parameters essential during coal utilisation as out lined in the methods section.

Gasification gave less gaseous emissions as compared to direct combustion mainly because the syngas produced during gasification is at higher pressure and temperature when compared to the exhaust gases produced during combustion. Also, the high pressure and temperature allow for easier removal of nitrogen and sulfur oxides, as well as trace elements contaminating the syngas [20]. Less air will be required for gasification process with minimal sulfur absorbed in ash. During gasification some of the sulfur in coal can either be absorbed by the limestone making up the reactor bed or turned to valuable chemicals like $H_2S$ and $H_2SO_4$[21].

### *Ash analysis*

The major elements contained in ash were silicon, aluminium, calcium and iron oxides, Table 3. The results were in agreement with those attained by [22, 23, 24]. The studies revealed that the mineral constituent is mainly made up of Si, Al, Fe and Ca oxides while elements such as Zn, Sr, Ti, S and others occur as minor constituents.

Table 3: Ash elemental analysis

| Element | Weight (%) | Element | Weight (%) |
|---|---|---|---|
| $Al_2O_3$ | 14.85 | Cr | 0.0219 |
| $SiO_2$ | 32.38 | Zn | 0.0113 |
| $P_2O_5$ | 0.4661 | Rb | 0.0031 |
| $K_2O$ | 0.5519 | Sr | 0.0884 |
| CaO | 14.33 | Y | 0.0066 |
| $TiO_2$ | 1.08 | Zr | 0.0563 |
| $Fe_2O_3$ | 9.23 | Nb | 0.0028 |
| MnO | 0.1139 | Sn | 0.0012 |
| Ba | 0.1028 | Pb | 0.0075 |
| Ta | 0.0076 | Th | 0.0031 |
| S | 2.05 | Cu | 0.108 |

The only discrepancies were in the percentage weight for silicon and aluminium oxides which were found to be below the range stated in other studies. These discrepancies may be attributed to preparation of the samples for the analysis. It has been noted that it is essential to ensure that there is no loss of important elements during the ashing procedure that can be brought about by high temperatures. The samples were subjected to high temperatures, around 1000°C, during the ashing procedure.

Examined deposits indicated that coal from Morupule Colliery has low tendency to fouling and slagging as shown by their respective indices in Table 4.

Table 4: Chemical parameters of coal deposits

| Deposit | Content |
|---|---|
| Ash content, $A^d$ (%) | 23 |
| Alkalinity/acidity (%) | 0.499 |
| Slagging Index | 0.374 |
| Fouling Index | 0.275 |
| Alkali Index | 0.126 |

According to Bielowicz [11] high aluminium silicate content and low the iron and alkali content (Ca, Fe, $K_2O_5$,$Na_2O$) correlates with a high melting point of ash hence a lower tendency to fouling. Ash analysis for coal sample under investigation revealed more aluminium and silicate content but less iron and alkali content (Table 4) hence basing on research work by Bielowicz[11], it can be concluded that the ash melting point will be high. High ash melting point prevents damage to combustion and gasification equipment as there will be no material hindering with air circulation and sticking to unburnt coal, thus increasing the furnace thermal efficiency[11].

## Numerical simulation analysis

The geometry mesh in Figure 1 was done with tetrahedral cells having 21 889 nodes and 105 467 cells.

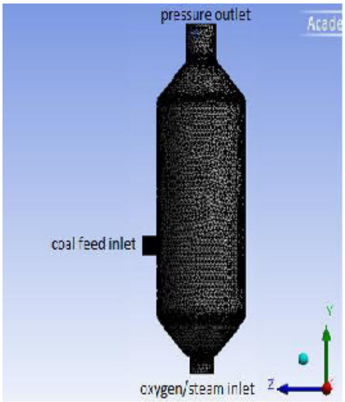

Figure 1: Meshed geometry of the gasifier

Empirical formula for the coal sample used in the study

$CH_{0.6}O_{0.1}S_{0.003}N_{0.02}$

Coal gasification reaction

$$CH_{0.6}O_{0.1} + 0.5O_2 + 0.5H_2O \rightarrow 0.01H_2 + 0.14CO + 0.09\,CO_2 + 0.24CH_4 + 0.44H_2O + 0.07C_6H_6$$

Simulation results attained minimum fluidisation velocity of 0.97m/s, terminal velocity of 1.5m/s and Reynold's number of 2.4exp07.

### Flow of gaseous fuels in the reactor

The simulation results in Figure 2 indicate spatial concentration of gaseous species in the reactor.

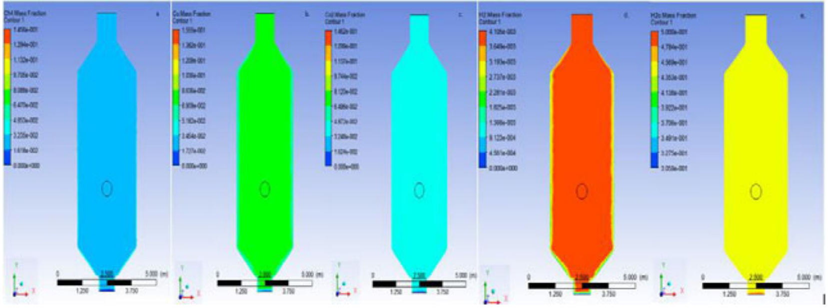

Figure 2: Species concentration in the gasifier

There was more hydrogen flowing inside the reactor as compared to other combustible gases. This was followed by CO. $CH_4$ was the least produced. High $H_2$ concentration could be due to the amount of CO in the reactor. It has been reported that increased CO concentration initiates $H_2$ production [25]. Low $CH_4$ production may be due to the fact that $CH_4$ is formed mainly during pyrolysis [25]. The results are in agreement with those from other studies [26-28] for $CH_4$, CO and $H_2$. The disagreement was for $CO_2$ concentration and this could be attributed to the kinetics used. Studies done by Wen et.al [29] and Stark et.al [30] indicated that gasification products making up the gas phase are mainly dependent on the kinetics used. The present study used two-competing rates model while the other studies used a comprehensive gas phase mechanism encompassing secondary pyrolysis, cracking and oxidation reaction of devolatilization process.

High pressures as shown in Figure 3a were experienced in the reactor due to devolatilization, combustion and gasification processes. It is suggested that the bombardment of molecules with the reactor walls and their interaction with each other (collisions) during those sub-processes resulted in increased pressure [31]. The elevated pressure led to low gas velocity in the reactor increasing towards the exit as the pressure lessened. The increase in velocity towards the exit was due to gas molecules getting lighter as the pressure on them reduced and the gasification process continued.

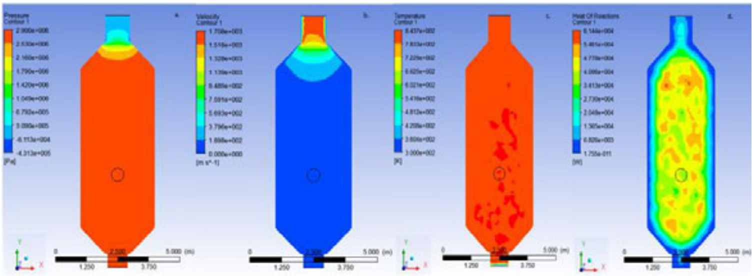

Figure 3: Pressure, velocity, temperature and heat of reactions distribution

The temperature was relatively high in the centre and bottom of the reactor as can be seen by the red markings in Figure 3c. High temperatures at the reactor bottom were due to the endothermic char gasification reactions as minimum fluidization velocity was attained [31]. It decreased in other parts of the reactor due to exothermic char gasification reactions and coal devolatilization process. The contours for heat of reactions show that more heat was produced towards the centre (1.97MW) of the reactor thus validating the temperature increase in the centre. In addition, heat due to reactions was also generated in the middle and bottom of the reactor because convectional currents were concentrated in those areas of the reactor due to low velocity. The results were in agreement with those obtained by Jones et.al [32] and Fernando [31].

### *Gasification Efficiency and Yield*

Gasification efficiency of 72% and gas yield of 0.696m$^3$ of synthetic gas was obtained for every kilogram of coal loaded into the gasifier each second. The efficiency agrees with the predicted values for coal gasification systems of 43% and above[20]. It also validates the little impact on gasification equipment by ash fouling and slagging i.e. the more fouling and slagging made by coal the less efficiency generated from the system.

## CONCLUSION

Coal from Morupule Colliery is medium volatiles bituminous with 23MJ/Kg of calorific value. The high calorific value is an indication of how effective it will be for power generation as less amount of coal will be required per unit of electricity. Also, there will be no need for back-up of fuel support since the calorific value will be sufficient to maintain good flame stability performance when operating at low loads. Data from combustion analysis indicate that when used for coal gasification technology, it will cause less damage to the equipment as it showed low tendency to fouling and slagging. Although the coal contains high sulfur, it can be used for a fluidized bed gasification technology. The limestone making up the bed of a fluidized bed reactor precipitates out sulfur during combustion thus reducing the amount of sulfur given out as sulfur dioxide.

The numerical simulation of coal gasification process was done to establish the flow and evolution of gaseous fuels in the reactor. Most of the carbon contained in coal was converted to gaseous fuels leading to enough syngas gas yield for further downstream process. It also indicated good system efficiency and gas yield both of which essential in power generation using Integrated Gasification Combine Cycle process. From the results of the study, it can be concluded that the coal under study has good properties for coal gasification technology.

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