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**Original Research Article**

## Steady State Simulation of Coal Gasification in a Fluidized Bed Gasifier

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**ABSTRACT**

*Gasification provides an important route for the conversion of coal to synthesis gas for the production of fuels, chemicals or for use in thermal power generation. Among the coal gasification processes, the fluidized-bed process with inherent advantage of high heat transfer and easy handling of solids is a natural choice. This work presents the steady state simulation of coal gasification in a fluidized bed gasifier using Aspen Plus 3.2. Data on the proximate and ultimate analysis for the coal and an assumption that major gasification reactions go to equilibrium was utilised to carry out the simulation. Sensitivity analysis was carried out to investigate the effect of various parameters such as temperature, pressure, steam to coal ratio and oxygen to coal ratio, on the syngas composition and the fraction of carbon left in the char. Results obtained were found to agree fairly well with experimental values, with slight over-prediction in the composition of hydrogen and slight under-prediction in the case of methane composition.*



## 1. INTRODUCTION

Increasing demand in global energy coupled with increasing oil prices has led to a search for alternative and sustainable energy resources (Bhutto et al., 2013; Odeh, 2015a; 2015b; 2015c). Among different alternatives, Synthetic gas (syngas) is on the lead in the search for alternative and sustainable energy and has been shown to be a favorable option resources (Shabbar and Janajreh, 2013; Olateju and Kumar, 2013, Tay et al., 2013; Vascellari et al., 2013; Lee et al., 2014; Odeh, 2015b). Synthesis gas (syngas) is considered as a clean fuel with environmental advantage compared to other fossil fuels because the sulfur oxides ($SO_X$) and nitrous oxide ($NO_X$) and carbon dioxide ($CO_2$) emissions are considerably lower (Lee et al., 2014; Odeh, 2015a). Coal gasification is a promising way to obtain syngas because the production techniques have achieved maturity and are commercially available (Odeh, 2015a; Odeh, 2015c). Moreover, the relatively high global resources of coal and its widespread availability worldwide make this resource a promising option (Odeh, 2015b). Two thirds of the total fuel fossil reserves in the world is coal and it will last for more than 150 years (Chejne and Hernandez, 2002; Odeh, 2015a). Gasification is a process that converts carbonaceous materials such as fossil fuel and biomass into a mixture of mostly hydrogen and carbon monoxide (called synthesis gas) (Grabner et al., 2007). Other gaseous species (including some potential air pollutants) are also formed; and the amounts depend on the fuel composition and process conditions (Nemtsov and Zabaniotou, 2007). The feedstock is combusted with insufficient oxygen to convert all the energy contained in the fuel into chemical energy in syngas (de Souza-Santos, 1989; Vascellari et al., 2013). The steam-oxygen gasification (SOG) process is the only commercialized method used to manufacture several chemicals from coal (Vascellari et al., 2013).

Aspen Plus has been widely employed to simulate chemical processes in a wide number of fields including but not limiting to the petroleum industry, chemical processes and biomass gasification (Duan et al., 2015). It can also be used to model steady state processes handling solid carbon materials in multiple unit operations. Therefore, many coal and biomass conversion processes have been simulated using Aspen Plus (de Souza-Santos, 1989; Duan et al., 2015; Verma and Kumar, 2015). Additionally, proximate and ultimate analysis properties of solids are specified to provide a fairly rigorous simulation of the gasification simulation process.

The aim of this work is to simulate and analyze the effect of operational variables viz temperature, pressure, steam to coal ratio, oxygen to coal ratio, on the composition of syngas. The knowledge obtained from this work will assist plant designers in the coal utility sector in the building of new reactors and the retrofitting of existing reactors for optimal performance.

## 2. METHODOLOGY

Aspen Plus software is one of the simulation package present in the Aspen Engineering Suite. This software was developed by AspenTech Int. Inc. Aspen Plus simulator gives a complete and integrated solution to a chemical process, thus providing an opportunity to check the feasibility of the process, to study and investigate the effect of various operating parameters on the entire process. It is a strong tool for simulation studies and helps in analyzing the outcome of the process. In this work, the Aspen Plus 2006, version 3.2 simulation package was used to simulate the process of coal gasification. The Aspen Plus simulation package was selected for modeling the fluidized bed gasification process because of the following reasons:

(1) Its capability to define non-conventional components in terms of their ultimate and proximate analysis and has an extensive built in physical database which can be used in all simulation calculations.
(2) Its capability of solids handling. As the introduction of solids in a process changes the heat and mass balances, even if the solids essentially pass through the process as an inert component. Aspen Plus include particular property model that accurately represents the solid particles.

### 2.1. Defining Components and Property Package

Components in Aspen Plus are classified as either conventional or non-conventional. Conventional components are ones with property data contained in Aspen Plus component database. These components such as $CO_2$, $H_2$, CO, $H_2O$, $CH_4$, $N_2$, $O_2$, etc., are directly added from the component database, into the component list during the simulation. The Soave-Redlick-Kwong property method was selected to calculate all the thermodynamic properties for the conventional components in the overall process. This thermodynamic model was chosen as it provides high accuracy in water-hydrocarbon systems over wide range of temperature. Non-conventional components are non-homogeneous substances that do not have a consistent composition and are not contained in the Aspen Plus component database. These components such as coal must be given physical attributes, such as those defined by the conventional coal analyses (ultimate and proximate and sulfur analysis). In Aspen Plus these exists as PROXANAL, ULTANAL AND SULFANAL. PROXANAL is the proximate analysis of the component where moisture, fixed carbon, volatile matter and ash are specified. ULTANAL is the ultimate analysis of the coal and contains the elemental composition of the coal. SULFANAL analysis differentiates between various forms of sulphur that is the non-conventional item. Property methods must also be chosen to calculate the enthalpy and density of the substance. In this work, the property methods HCOALGEN and DCOALIGHT were respectively chosen to calculate the enthalpy and density of the coal. These property methods use statistical correlations to calculate the specific heat, the enthalpy and density of the coal, based on the ultimate, proximate and sulfur analysis. The following are the list of components selected in this simulation and their class:

- COAL (Non-Conventional)
- ASH (Non-Conventional)
- C (Solid)
- $H_2$ (Conventional)
- $H_2O$ (Conventional)
- CO (Conventional)
- $CO_2$ (Conventional)
- $CH_4$ (Conventional)
- $C_2H_6$ (Conventional)
- $N_2$ (Conventional)
- $O_2$ (Conventional)
- $NO_2$ (Conventional)
- $NO_3$ (Conventional)
- S (Conventional)
- $SO_2$ (Conventional)
- $SO_3$ (Conventional)
- $H_2S$ (Conventional)

**2.2. Selecting Stream Class**

Because the decomposition of coal forms carbon, a stream class that includes conventional solids is used. In this simulation the MCINCPSD stream class was used. MCINCPSD stream class contains the following sub streams:

- MIXED
- CIPSD
- NCPSD

The MIXED sub stream contains the conventional non-solid components selected in the simulation, present in the main stream class. CIPSD sub stream contains the conventional solid selected in the simulation, present in the main stream class (MCINCPSD). In this work, solid carbon (C) belongs to the CIPSD sub stream class. The NCPSD sub stream contains the non-conventional solid components present in the main stream class. In this paper, coal and ash belongs the NCPSD sub stream.

**2.3. Simulation Model Description**

Coal gasification models can be divided into two:

1. Kinetic model which defines the complex kinetics of the reactions by specifying their rate expressions, rate constants, activation energies and Arrhenius constants. The simulator solves for the concentrations of the reacting species at the specified residence time under the predefined reaction conditions.

2. Equilibrium model which predicts only end reaction product distribution but gives no idea about the instantaneous product distribution along the geometric dimensions.

In this particular simulation an equilibrium model was utilized. The following assumptions were considered in modeling the gasification process:

1. The process is isothermal and operates under steady state conditions.
2. The gasifier is perfectly insulated, meaning that; heat losses are negligible.

3. Coal devolatilization takes place instantaneously and volatile products mainly consist of $H_2$, CO, $CO_2$, $CH_4$, and $H_2O$.
4. The residence time for reactants is sufficiently high for both devolatalization and char combustion reactions to reach equilibrium.
5. All the sulphur is the feedstock reacts to $H_2S$, only $NH_3$ is formed and no nitrogen oxide is considered.
6. Tar and heavy hydrocarbons are products of non-equilibrium reactions and thus are not considered in this model.

For the purpose of simulation, the fluidized bed gasifier was considered to have two distinct zones:

1. Drying / Devolatilization (Pyrolysis) zone
2. Combustion / Char gasification zone.

### 2.3.1. Drying/devolatilization (pyrolysis)

The dried coal feed (DRYCOAL), specified as a non-conventional solid is first converted into its constituting elements (C, H, O, N, S and ASH) and moisture ($H_2O$). This decomposition of the coal is accomplished by the RYIELD reactor, labeled DECOMP, which is a reactor model that generates products based on the component yield specification as obtained from the ultimate analysis and this determines the mass flowrate of each component in the RYIELD reactor block outlet stream (DECOMP). The carbon content of the DRYCOAL feed is converted to solid carbon graphite. The hydrogen, oxygen, nitrogen, chlorine and sulfur are converted to gaseous $H_2$, $O_2$, $N_2$, $Cl_2$ and S. Finally, the moisture content is converted to liquid $H_2O$. During pyrolysis, the carbonaceous material, coal in this instance, is heated enough that it decomposes into volatile constituents. Pyrolysis is coal burning in the abseence of oxygen (i.e. burning of coal without the presence of external oxygen source) and the extraction the volatile components from the coal, leaving behind a solid residue, which is a carbon rich source (this solid residue is reffered to as char). To model this process, a separator block (SEPARATE) was introduced to split the carbon present in the coal, since carbon partly constitutes the gas phase which takes part in devolatilization (pyrolysis), and the remaining carbon comprises part of the solid phase (char) and subsequently undergoes char gasification. The fixed carbon content goes into the CHAR stream as residue left from pyrolysis while the free carbon takes part in pyrolysis reaction $H_2$, $O_2$, $N_2$, $Cl_2$ and S to from volatile compounds; $H_2$, $CH_4$, $H_2O$, CO and $CO_2$. The pyrolysis reaction was modeled with the RGIBBS reactor model (PYROREAC), with the assumption that the pyrolysis reactions follow the Gibbs equilibrium conditions. The RGIBBS equilibrium reactor model does not accept non-conventional components such as coal as reactants. This was the reason for the decomposition of the coal into conventional components which can be used by the RGIBBS reactor block.

### 2.3.2. Combustion/char gasification

In the presence of steam and oxygen, volatile matter undergoes combustion while char undergoes combustion and gasification. The VOLAT and CHAR streams are fed to a mixer and combined with oxygen and steam. The mixer outlet stream goes into another RIGIBBS reactor block, named GASIFIER to model the combustion and char gasification reactions assuming these reactions go to equilibrium. The products from the GASIFIER are fed to a CYCLONE block to separate the solids present from the gas stream (RAWGAS).

Figure 1 shows the modeled flowsheet for the fluidized coal gasification used in this study. The ultimate and proximate analysis data, gasification operating conditions and stream operating conditions were obtained from previous study by Odeh (2015a) and are presented in Tables 1-5.

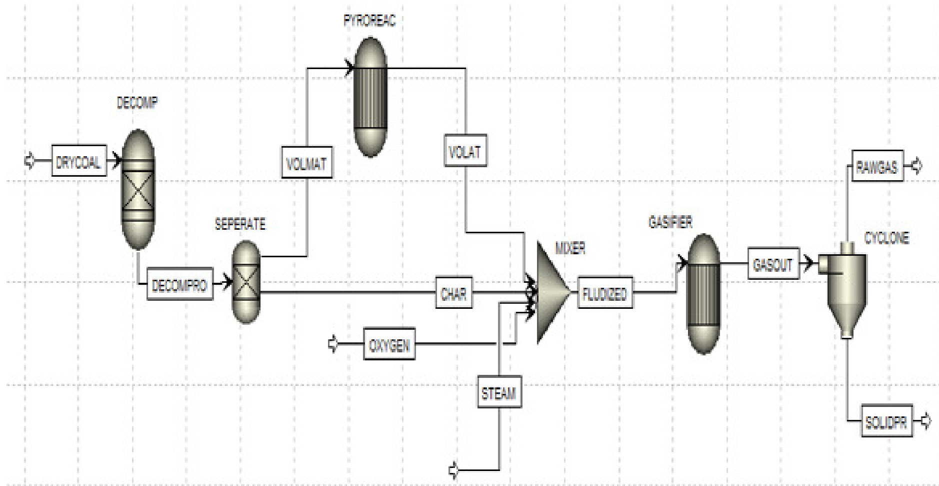


Figure 1: Flowsheet for the simulation

Table 1: Reacting conditions for the simulation process

| Operation | Blocks | Name | Operating conditions |
|---|---|---|---|
| Drying/Devolatilization (Pyrolysis) | RYIELD | DECOMP | 300 $^oC$, 1bar |
| Drying/Devolatilization (Pyrolysis) | SEPERATOR | SEPARATE | 300 $^oC$, 1bar |
| Drying/Devolatilization (Pyrolysis) | RGIBBS | PYROREAC | 700 $^oC$, 1bar |
| Combustion/Char gasification | MIXER | MIXER | 900 $^oC$, 1bar |
| Combustion/Char gasification | RGIBBS | GASIFIER | 1100 $^oC$, 1bar |
| Combustion/Char gasification | CYCLONE | CHARSEP | 1100 $^oC$, 1bar |

Table 2: Stream conditions of the simulation process

| STREAMS | Operating conditions |
|---|---|
| DRYCOAL | 5 kg/s, 75 $^oC$, 1bar |
| STEAM | 2.5 kg/s, 500 $^oC$, 1bar |
| OXYYGEN | 1 kg/s, 200 $^oC$, 1bar |

Table 3: Ultimate analysis

| Elements | C | H | N | Cl | S | O |
|---|---|---|---|---|---|---|
| Wt% d.b. | 66.9 | 4.9 | 1.1 | O.1 | 1.3 | 16.5 |

Table 4: Proximate analysis

| Components | Volatiles | Fixed C | Ash |
|---|---|---|---|
| Wt% d.b. | 45.9 | 44.9 | 9.2 |

Table 5: Sulfur analysis

| Component | Pyrite S | Sulfate S | Organic S |
|---|---|---|---|
| Wt% | 0.02 | 0.02 | 0.02 |

## 3. RESULTS AND DISCUSSION

### 3.1. Effect of Gasification Temperature on Syngas Composition

The effect of gasification temperature on the composition of the synthesis gas, obtained from the simulation is presented Figure 2.

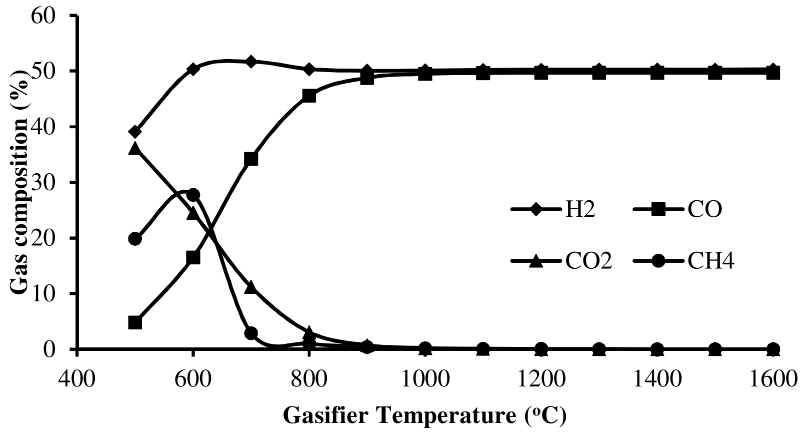


Figure 2: Effect of gasification temperature on syngas composition (Steam to Coal ratio = 0.5, Oxygen to Coal = 0.2, Gasification pressure = 1bar)

From Figure 1, it can be seen that the composition of hydrogen and methane increased with increasing gasifier temperature, up to about $600^0$C, then after, increasing gasifier temperature led to a decrease in the methane composition and a small increase in hydrogen composition, before arriving at a temperature-independent hydrogen composition. It was also observed that the composition of carbon monoxide increased, while the composition of carbon dioxide decreases, with increasing gasifier temperature. The reason for the increase in $H_2$ and $CH_4$ compositions in the syngas when gasifier temperature increased to about $600^0$C is as a result of the char gasification reactions given in Equations 1 and 2, which are favored at such temperatures.

$$C + H_2O \rightarrow CO + H_2 \quad (1)$$

$$C + 2H_2 \rightarrow CH_4 \quad (2)$$

At higher temperatures above 600 °C, the composition of methane dropped drastically while that of hydrogen increased a little before attaining a constant, temperature-independent composition of about 50%. This could be attributed to the fact that, at such higher temperatures, cracking of methane into carbon and hydrogen starts to occur, leading to a decrease in methane composition and an increase in hydrogen composition as presented by Equation (3) (Duan et al., 2015).

$$CH_4 \rightarrow C + 2H_2 \quad (3)$$

It was also observed that increasing the temperature of the gasifier increased CO composition and decreased $CO_2$ composition. The reason for this is that as temperature increases, char gasification reactions are favored as illustrated by Equations (4) and (5) (Verma and Kumar, 2015).

$$C + H_2O \rightarrow CO + H_2 \quad (4)$$

$$C + CO_2 \rightarrow 2CO \quad (5)$$

More so, at higher temperatures, the water gas shift reaction inclines towards CO and $H_2O$ production as shown in Equation (6) (de Souza-Santos, 1989). This is because the water gas shift reaction ($CO + H_2O \leftrightarrow CO_2 + H_2$) is an exothermic one and an increase in temperature favors the backward reaction, according to Le Chatelier's principle.

$$CO + H_2O \leftarrow CO_2 + H_2 \quad (6)$$

### 3.2. Effect of Gasification Pressure on Syngas Composition

The effect of gasifier operating pressure on the composition of the syngas produced from the simulation is shown in the Figure 3.

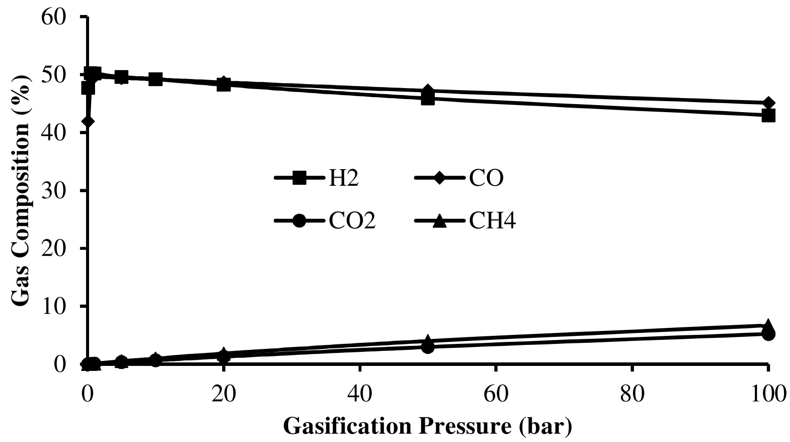


Figure 3: Effect of gasification pressure on Syngas composition (Steam to coal ratio = 0.5, Oxygen to coal = 0.2, Gasification Temperature = 1100 $^oC$)

From Figure 3, it was observed that as the gasifier pressure increases, CO and $H_2$ in syngas composition decreases while $CH_4$ and $CO_2$ in syngas composition increases. The can be explained using Le Chatelier's principle and the consideration of the following gasification reactions:

$$C_{(s)} + CO_{2\,(g)} \leftrightarrow 2CO_{(g)} \quad (7)$$
$$C_{(s)} + H_2O_{(g)} \leftrightarrow CO_{(g)} + H_{2\,(g)} \quad (8)$$
$$C_{(s)} + 2H_{2\,(g)} \leftrightarrow CH_{4\,(g)} \quad (9)$$
$$CH_{4\,(g)} + H_20_{(g)} \leftrightarrow CO_{2\,(g)} + 3H_{2\,(g)} \quad (10)$$
$$CO_{(g)} + H_2O_{(g)} \leftrightarrow CO_{2\,(g)} + H_{2\,(g)} \quad (11)$$

According to Le Chatelier's principle, for a change in pressure to affect a system in equilibrium:

- one of the reactants or products in the reversible reaction must be gaseous
- the total number of moles of gaseous molecules on the left side of the equation must be
- different from the total number of moles of gaseous molecules on the right side.

If a high pressure is applied to an equilibrium system, the reaction which involves a reduction in pressure will be favored. Conversely, if a low pressure is imposed on an equilibrium system, the reaction which results in an increase in pressure will be favored. By implication, increasing gasification pressure would:

- favour the formation of $CO_2$ and C and reduce the formation of CO in reaction
- Equation 7
- favour the formation of $H_2O$ and C and reduce the formation of CO and $H_2$ in reaction Equation 6
- favour the formation of $CH_4$ and reduce the formation of $H_2$ and C in Equation 9
- favour the formation of $CH_4$ and $H_2O$ and reduce the formation of $CO_2$ and $H_2$ in reaction Equation 8

- have no effect on reaction Equation 11

The overall effect would lead to an increase in methane and carbon (iv) oxide compositions in the syngas and a decrease in the carbon (ii) oxide and hydrogen compositions in the syngas. From Figure 3, it can also be observed that significant change in syngas composition with pressure occurs at extremely high pressures and this is in agreement with what is reported in (Verma and Kumar, 2015)

### 3.3. Effect of Oxygen to Coal Ratio on Syngas Composition

The composition profile of individual specie in the syngas with increasing oxygen to coal ratio is shown in the Figure 4.

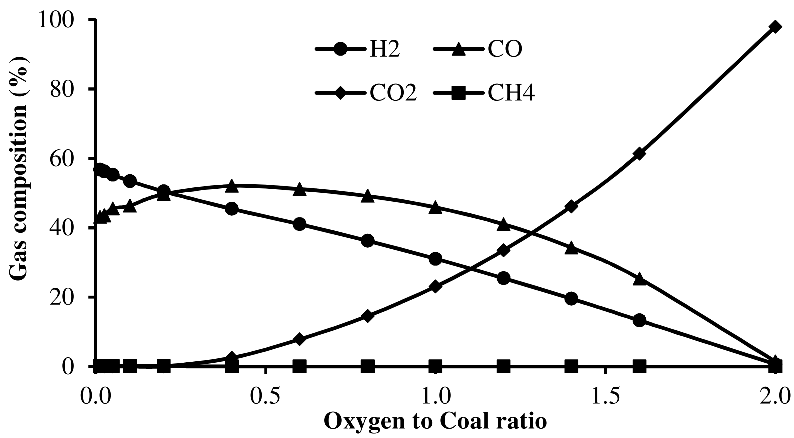


Figure 4: Effect of oxygen to coal ratio on syngas composition (Steam to coal ratio = 0.5, Gasification temperature = 1100 °C, Gasification pressure = 1bar)

Figure 4 shows that an increase in the oxygen to coal ratio resulted in an increase in $CO_2$ composition and a decrease in the composition of $H_2$ and CO. This is attributed to the oxidation of $H_2$ to $H_2O$ and expressed in Equation 12.

$$H_2 + O_2 \rightarrow H_2O \qquad (12)$$

As the oxygen to coal ratio increases, the composition of CO increased to a maximum (region of partial oxidation) and began to drop (region of complete oxidation) until its composition became zero at oxygen to coal ratio of 2.0. Also, the composition of $CO_2$ was found to increase as the oxygen to coal ratio increased. This is as a result of complete oxidation (Nemtsov and Zabaniotou, 2008).

$$2CO + O_2 \rightarrow 2CO_2 \qquad (13)$$

$$C + O_2 \rightarrow CO_2 \qquad (14)$$

$$CH_4 + O_2 \rightarrow CO_2 + H_2O \qquad (15)$$

### 3.4. Effect of Steam to Coal Ratio on Syngas Composition

The effect of steam to coal ratio on the composition of the syngas is presented in Figure 5.

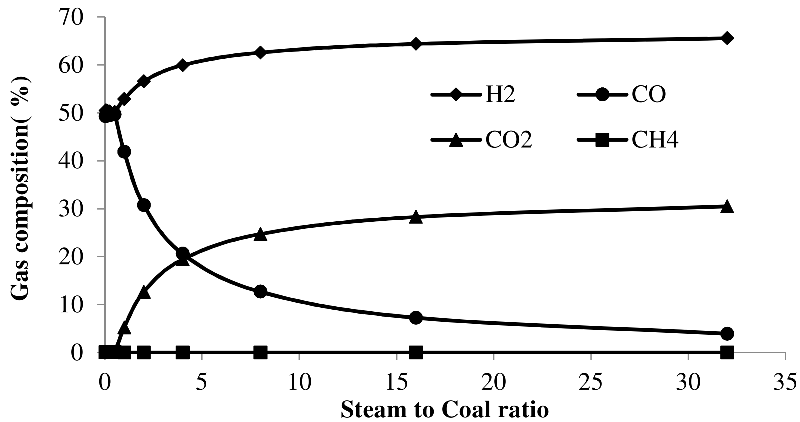


Figure 5: Effect of Steam to Coal ratio on Syngas composition (Oxygen to coal = 0.2, Gasification Temperature = 1100 °C, Gasification pressure = 1bar)

It was observed that as the steam to coal ratio increased, $CO_2$ and $H_2$ in the syngas composition increased, while CO composition decreased until an independent steam to coal ratio compositions were attained for the various species. This effect is as a result of steam gasification reactions which are predominating in excess of steam (Grabner et al., 2007; Duan et al., 2015).

$$CH_4 + H_20 \leftrightarrow CO_2 + 3H_2 \quad (16)$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (17)$$

## 4. CONCLUSION

In this work, fluidized bed coal gasification was simulated using Aspen Plus to estimate syngas composition. The simulation was performed on a known composition of a coal sample using its proximate and ultimate analysis and the effect of various operating parameters on the product gas composition. Results obtained revealed product composition that corroborates experimental results of other researchers. As such, information from this work serves as a tool capable of handling different types of coal feed streams in order to produce syngas. To be best of the authors knowledge, the application of simulation (Aspen Plus) to coal gasification in this era of clean coal technology is novel.

## 5. CONFLICT OF INTEREST

There is no conflict of interest associated with this work.

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