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Sensitivity Analysis and Parametric Optimization of Hydrogen Production from Afuze Coal through Air-Steam Gasification

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Abstract

Coal is a carbon-rich sedimentary rock and fossil fuel that accounts for over 60% of all economically recoverable primary sources of energy on earth. The burning of coal emits ~40% of the entire energy-related atmospheric greenhouse gases, which poses risks to human health, safety, and the environment. Given this scenario, there are growing concerns about the long term sustainability of the industry vis-à-vis its effects on global warming and climate change. However, clean technologies such as gasification with carbon dioxide capture could be the panacea to the challenges of coal-fired electricity generation. Therefore, this study investigates the hydrogen (H_2) and syngas potential of Afuze (AFZ) coal earmarked for electricity generation in Nigeria. Consequently, the mathematical simulation, sensitivity analysis, and optimization of AFZ were performed under air-steam gasification conditions using ASPEN Plus. Results revealed that AFZ gasification from 200°C to 1600°C and the feed rate of 1000 kg/h yields H_2, CO, CO_2 and CH_4. The optimal conditions for H_2 and syngas were observed at 950°C, ER = 0.31 and SC = 2.0 at the optimal gas compositions of H_2 (48 mol.%), CO (11 mol.%), CO_2 (11 mol.%) and CH_4 (0 mol.%). Furthermore, temperature (T), equivalence ratio (ER), steam to carbon (SC) ratio greatly influenced AFZ gasification, whereas pressure did not impact the process. In conclusion, bench-scale or demonstration gasifier tests are required in future AFZ gasification studies to comprehensively investigate its energy recovery and electricity generation potentials.

Keywords: *Sensitivity analysis; Optimization; Hydrogen;Afuze coal; Air-Steam gasification.*

1. Introduction

Coal is the most abundant and dispersed fossil-based fuel on the planet [1-2]. It accounts for over 60% of all economically recoverable sources of primary energy on earth [3]. Over the years, coal has become an integral part of the global energy mix, which accounts for ~38% or about 8,000 TWh of the entire electricity generated worldwide [3-4]. The burning of coal for electricity generation in power plants is largely based on pulverised coal combustion, which causes numerous socio-economic and environmental problems [5-6]. Coal-fired electricity generation emits ~40% of the entire energy-related greenhouse gases found in the atmosphere [7-8].

Various studies have shown that the process is responsible for land degradation and the pollution or poisoning of water sources [9-10], which endangers human health, safety, and the environment.

The outlined problems have also raised concerns about the long term sustainability of coal-fired power generation due to its effects on global warming and climate change. Hence, there is a growing resistance to coal utilization. Given this scenario, numerous financiers, governments, and social campaign groups have called for the outright ban, rollback of funding and or the cancellation of future coal projects [11-12]. However, the growing demand for cheap electricity particularly in countries characterised by energy poverty is expected to increase future coal demand. Likewise, the discovery of coal deposits in emerging nations (e.g. Mozambique, Viet Nam, Cambodia and Nigeria) suggest coal could remain a prominent part of the global energy mix [13-14].

The adoption and implementation of cleaner coal technologies have been proposed by scientists to mitigate the growing environmental concerns and problems of coal power generation [15-16]. Typically, the concept of clean coal advocates for reduced coal consumption, efficient conversion, and mitigation of emissions from coal-fired power plants. Examples of technologies proposed over the years include; near-zero-emissions and highly efficient and low emissions (HELE) power plants that utilize carbon capture utilization and storage (CCUS) technologies [17-19]. Other examples include; flue gas desulfurization, selective catalytic reduction, and electrostatic precipitators [20-21]. Among the outlined technologies, gasification is considered one of the most promising technologies for thermochemical conversion along with the amelioration of the harmful effects of coal utilization [22-23]. It is typically considered an environmentally friendly technology for the conversion of low value and carbon-based raw materials such as coal into high-value synthesis gas (syngas), energy, fuels, and chemicals [24].

Over the years, numerous gasification related technologies such as underground coal gasification [25-26], co-gasification (biomass/coal) [27-28], ultra and supercritical water gasification [29-30], and integrated gasification combined cycle (IGCC) [31-32] have been reported in the literature. Other studies have examined the potential energy recovery, product gas yield and distribution, pollutant emissions, kinetics and optimisation of coal gasification through mathematical modelling software such as ASPEN Plus [33-35]. The findings showed that ASPEN Plus is a practical, cost-effective and reliable tool for modelling the product gas, yield, and composition of different coal ranks for enhanced energy recovery. Furthermore, ASPEN can be used to simulate the optimal operating conditions, engineering economics, and pollutant emissions of coal conversion.

Therefore, the objective of this study is to model the parametric air steam gasification of Afuze (AFZ) coal using ASPEN Plus. The study will also present findings on the product gas yield, composition, sensitivity, and optimisation of the AFZ coal acquired from the Owan East Local Government Area in the Edo State of Nigeria. The selected operational parameters for the mathematical simulation AFZ coal air-steam gasification conditions in ASPEN Plus will be coal feed rate, air flow rate, temperature, pressure and steam to carbon (SC) ratio. Previous studies have examined the physicochemical, mineralogical, microstructure, thermal and kinetic characteristics of AFZ coal [36-38]. However, the findings are limited to the estimated reserves, potential energy, and fuel characteristics of AFZ coal. To the best of the authors' knowledge, there is currently no published study on the product yield, gas composition, emission profiles, sensitivity and optimization analysis of AFZ coal gasification, despite advanced plans for its utilization for coal-fired power generation in Nigeria [39]. Hence, it is envisaged that the findings of the study will provide comprehensive data on optimal conditions and pollutant emissions for the design and operation of the planned coal plant.

2. Theory and methods

2.1. Theory

The process was modelled and simulated by Gibbs free energy minimisation of the components involved in the primary reactions of the gasification process. The reactions consist of water gas shift, steam reforming, and methanation. The governing equations for Gibbs free energy for *N* species (*i* = 1…*N*) are stated as follows [40]:

$$G_{total} = \sum_{i=1}^{N} n_i \Delta G_{f.i}^{0} + \sum_{i=1}^{N} n_i RT\, ln\left[\frac{n_i}{\sum n_i}\right] \quad (1)$$

The terms $\Delta G_{f.i}^{0}$ denote the Gibbs free energy of formation of the *i*th species at the standard pressure. The minimisation of the objective function was solved for n_i using Eq. 1. The carbon content, determined by ultimate analysis, should be equal to the total carbon content in the gas mixture. Therefore, the expression for *j*th element can be written as;

$$\sum_{i=1}^{N} a_{i,j}\, n_i = A_j \quad (2)$$

Here the terms $a_{i,j}$ describe the number of atoms of the *j*th element in the *i*th species and A_j is the total number of atoms of element *j* going into the reactor. Based on the Lagrange multiplier, the term λ methods is given by the relation:

$$L = G_{total} - \sum_{i=1}^{N} \lambda_j \left(\sum_{i=1}^{N} a_{i,j}\, n_i - A_j\right) \quad (3)$$

Consequently, the extreme points can be obtained by substituting Eq 3into Eq 1;

$$\frac{\partial L}{\partial n_i} = \frac{\Delta G_{f.i}^{0}}{RT} + \sum_{i=1}^{N} ln\left(\frac{n_i}{n_{total}}\right) + \frac{1}{RT}\sum_{j=1}^{K} \lambda_j \left(\sum_{i=1}^{N} a_{i,j}\, n_i\right) \quad (4)$$

In this study, the major products of steam reforming that were considered include; H_2, CO, CO_2, CH_4, C (graphite) and excess steam. The high carbon content of the reacting components was thus considered in this study. However, the potential secondary components considered include; ethane, ethylene, acetylene, and ethanol, which were previously reported as negligible in the literature [41]. In practice, the presence of secondary products even at low concentrations is considered the precursor of coke. The most common reactions during steam reforming of coal include; methanation, water gas shift, and steam reforming reactions as presented in Eq 5-7 [42]:

$$C_xH_yO_z + (x - z)H_2O \leftrightarrow xCO + (x + y/2 - z)H_2 \quad (5)$$

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

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \quad (7)$$

Combining Eq 5 and 6 results in the general reaction equation for the steam reforming of carbonaceous materials in the literature [42];

$$C_xH_yO_z + (2x - z)H_2O \leftrightarrow xCO_2 + (2x + y/2 - z)H_2 \quad (8)$$

The overall product gas yield consists of H_2, CO, CO_2 and CH_4, which are calculated from Eq. (8).

2.2. Process description

The coal gasification simulation process was developed in ASPEN Plus software. The flow sheet of the process that consists of a three-model unit: the RYield (DECOMP), RGibbs (BURN), Separator (SEPARATE) and Calculator unit is presented in Figure 1. The RYield block in the model was used to convert the proximate, ultimate, and sulphanal properties of the lignite coals (presented in Table 1) into potential chemical compounds. On the other hand, the Calculator module employed to normalise the output of the RYield which consists of water (H_2O), ash, carbon (C), hydrogen (H_2), nitrogen (N_2), chlorine (Cl_2), sulphur (S) and oxygen (O_2). Likewise, the outlined components serve as the inlet constituents for the RGibbs or gasification unit. The unit employed the Gibb free equilibrium analysis to calculate the moles of each reactor constituent at the stated operational settings. Apart from the inlet components from the RYield, the products in the RGibbs comprise the entire potential gas products of gasification. Typically, the products consist of hydrogen (H_2), carbon monoxide (CO), carbon dioxide

(CO_2), methane (CH_4) and ethylene (C_2H_4). Next, the products of the RGibbs unit were separated into gases and solid products of the gasification process using the stream separator block in ASPEN.

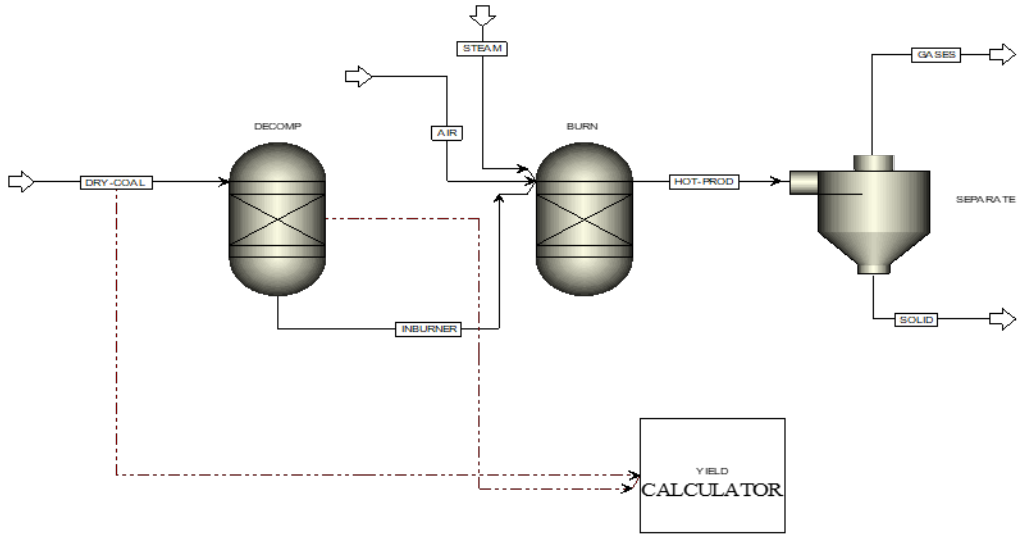

Figure 1. Flow sheet of coal gasification in ASPEN Plus

Table 1. Proximate, ultimate and sulphanate analysis of AFZ [43]

Analyses	Element	Symbol	AFZ (wt.%)
Ultimate	Carbon	C	50.0
	Hydrogen	H	4.2
	Nitrogen	N	1.1
	Chlorine	Cl	0.0
	Sulphur	S	1.0
	Oxygen	O	12.7
Proximate	Moisture	M	2.0
	Volatile Matter	VM	45.8
	Ash	A	31.0
	Fixed Carbon	FC	21.2
Sulphanal	Pyritic	S1	0.45
	Sulfate	S2	0.1
	Organic	S3	0.45

3. Results and discussion

3.1. Effect of temperature on AFZ gas composition

The gasification profile comprising the gas products composition at various temperatures is presented in Figure 2. The simulation was performed at a constant feed rate of 1000 kg/h of AFZ coal, Airflow of 15 kmol/h, steam flow of 1500 kg/h and pressure of 1 bar.

As observed, the content of H_2 increased from 0.0 mol-frac at 200°C to 0.52 mol-frac at 650°C, which was then followed by a decrease to 0.50 mole-frac at 1600°C. Similarly, the CO increased from 0.0 to 0.17 mol-frac at 200°C and 1600°C. The other gas composition CO_2 and CH_4 decreased with an increase in temperature from 200°C to 1600°C. The maximum content of CO_2 and CH_4 at 200°C was 0.26 and 0.16 mol-frac, whereas at 1600°C the values were 0.08 and 0.0 mol-frac, respectively. The optimal conditions were determined when H_2+CO (syngas) was greater than CO_2, which occurred at 950°C, 1 bar, ER = 0.31 and SC = 2.0. Consequently, the optimal gas composition (mol.%) for H_2, CO, CO_2 and CH_4 are 48%, 11%, 11% and 0%, respectively.

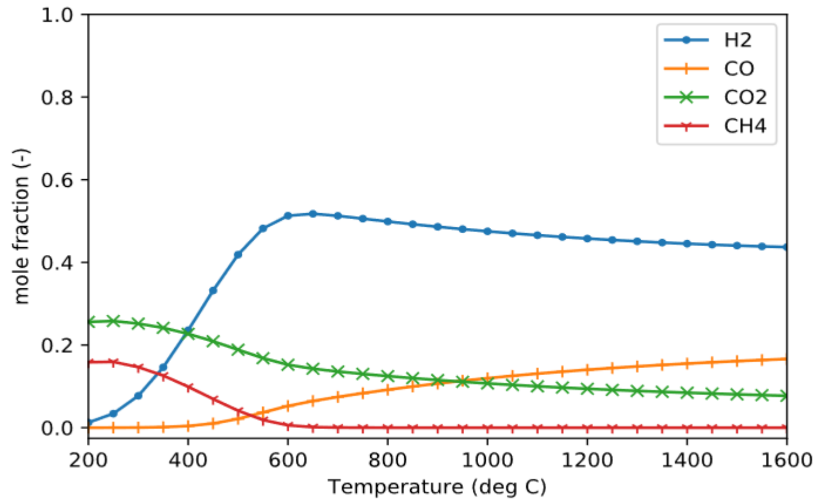

Figure 2. Profile of AFZ coal gasification gas product

3.2. Effect of ER and SC on H_2 composition

Figure 3 shows the sensitivity of H_2 composition to changes in the equivalence ratio (ER) and steam to carbon (SC) ratio for simulation of the AFZ feed at 1000 kh/h, 950°C and 1 bar. For ER value ≥ 1.0 combustion occurs whereas for values < 0.2 pyrolysis takes precedence. Therefore, the gasification range typically occurs in the range ER = 0.2-0.9. As observed, the profiles show that the composition of H_2 decreased with increasing ER, whereas the composition increased with an increasing ratio of SC. However, the entire profiles converged at ER = 1.03 for all values of S/C where the H_2 mol-frac is 0.0. Furthermore, the highest (57%) and lowest (34%) composition of H_2 within the gasification range occurred at ER = 0.21, and S/C values of 6.67 and 0.0, respectively. The optimal value of S/C was observed at 2.0 as determined by the last significant per cent change in gas composition. The H_2 composition at the optimal condition was 52 mol.%.

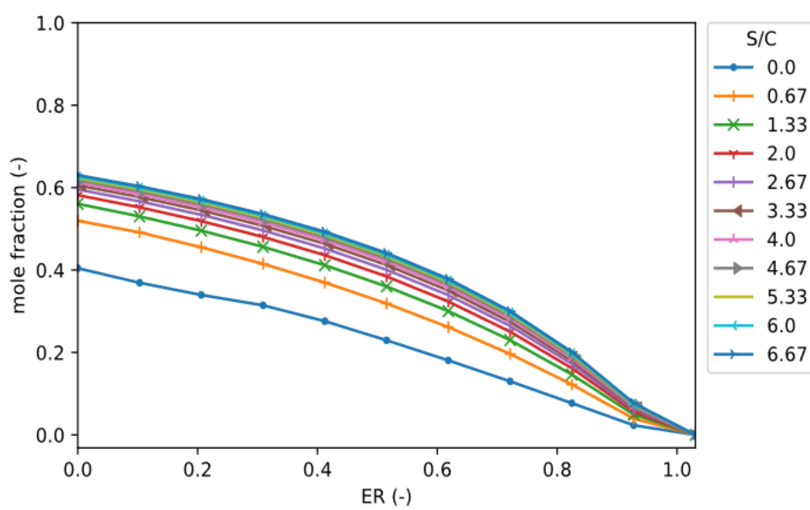

Figure 3. AFZ H_2 mole-fraction variation with ER and S/C

3.3. Effect of temperature and ER on H_2

Figure 4 presents the simulated sensitivity of H_2 composition during AFZ gasification under the conditions; 1000 kg/h feed rate, Airflow 15 kmol/h, and steam flow rate of 1500 kg/h. For the ER range 0.0 to 1.03 considered in this study, the H_2 composition started from 0.0 mol-frac at 200 °C and increased at the same rate from ER = 0.0 – 0.82 but peaked at a different

H_2 composition (0.21-0.60 mol-frac) with decreasing order in the range from 500°C to 700°C. As observed, the composition of H_2 is less sensitive to temperature for ER 0.93 and 1.03. However, when the ER for simulation reached maximum, the H_2 composition was almost flat and in some cases slightly reduced. Hence, the highest composition of H_2 in mol-frac is 0.60 at ER = 0.0 and temperature 700°C, where the lowest is 0.0 at 1.03, which are outside the gasification range.

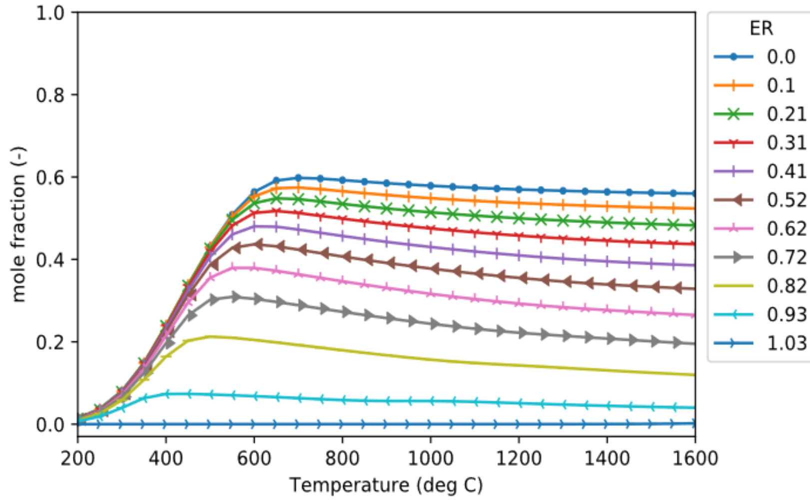

Figure 4. AFZ H_2 mol-frac variation with temperature and ER

3.4. Effect of pressure and ER on H_2

Figure 5 shows the sensitivity profile of the H_2 composition to gasification pressure. The simulation was performed at the conditions AFZ feed rate of 1000 kg/h, Steam flow rate of 1500 kg/h and temperature of 950°C. As observed, the composition of H_2 was constant for the pressures 1 – 25 bar considered but was found to increase with decreasing in ER. The profile shows that the production of H_2 during AFZ gasification is not sensitive to pressure. Therefore, the optimal pressure is 1 bar, which resulted in the maximum H_2 composition of 0.58 mol-frac at ER = 0.0, whereas the lowest (0.0) was at ER = 1.03.

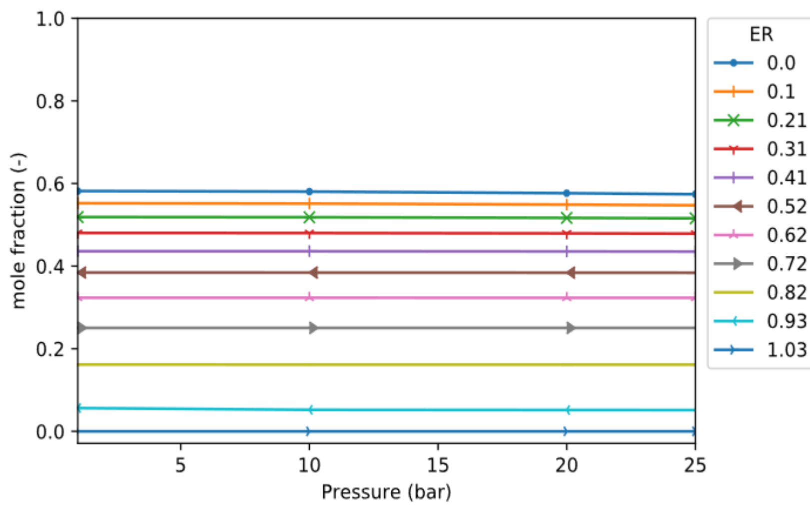

Figure 5. AFZ H_2 mole-fraction variation with pressure and ER

4. Conclusions

The study presents results of the successful mathematical simulation, sensitivity analysis and parametric optimization of hydrogen (H_2) and syngas production from Afuze coal earmarked for electric power generation in Nigeria. The mathematical simulation was performed using ASPEN Plus software under air-steam gasification conditions using coal feed rate, airflow rate, temperature, pressure and steam to carbon ratios as operational parameters. The findings showed that the product gas yield and composition of the AFZ coal consists primarily of H_2, CO, CO_2 and CH_4 as determined at the feed rate of 1000 kg/h, airflow 15 kmol/h, steam flow 1500 kg/h, atmospheric pressure, and temperatures from 200°C to 1600°C. The sensitivity and optimisation analyses revealed that the optimal conditions for H_2 and syngas are; 950°C, 1 bar, ER = 0.31 and SC = 2.0. Overall, the results showed that the parameters, namely; temperature (T), equivalence ratio (ER), steam to carbon (SC) ratio greatly influenced the yield and composition of H_2 and syngas produced, whereas the profiles showed that the air steam gasification of AFZ coal is not sensitive to pressure. In conclusion, the authors recommend that empirical tests are conducted using bench-scale or demonstration gasifiers to examine air steam gasification of AFZ coal for enhanced energy recovery and electric power generation through H_2 and syngas.

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