

KINETIC BASED SIMULATION OF FIXED BED GASIFIER.

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Abstract: Biomass is one of the most clean and renewable energy resources. Researchers give more and more attentions to the biomass because it can effectively reduce the amount of greenhouse effect due to its zero emission of carbon monoxide. From biomass utilization technologies, biomass gasification is an attractive mechanism for utilizing effectively. Despite the application of fixed bed flow gasification on larger scales; the reaction rates in the hot conversion zone are almost unknown. But the knowledge of the rates of the gasification reactions at high temperature and high pressure is crucial for the detailed design and optimization of the gasifier. This work was focusing on the simulation of the biomass (coffee bean husk and rice husk) gasification process based on the kinetics of the gasifier and to investigate the produced syngas composition. The ASPEN PLUS simulator was used to investigate the effect of operating parameters on composition of product gas.

Keywords: Fixed bed gasifier, biomass, equivalence ratio, ASPEN PLUS.

Introduction:

The price of oil and gas as well as the energy crisis are continuously rising; there is a growing demand for the energy which is environmentally friendly and low cost. Biomass is one of the most choices among these kinds of energy resources since it is abundantly available, renewable and environmental friendly [1]. And also there is near to zero CO₂ emission and lower NO_x and SO_x emission than fossil fuel [2]. Biomass gasification process has developed as a potential solution to rural electrification in developing countries through decentralized power generation. Biomass gasification is one of the most popular processes which produce energy in the form of syngas and as the same time it reduces the environmental hazards of raw biomass. In addition, being a renewable energy source, biomass gasification also helps reduction of net greenhouse gas emission and moderation of global warming [3]. Gasification is a thermochemical process that converts organic or fossil based carbonaceous material into a combustible gas by react the material under a certain range of temperature with a controlled/starved amount of air/oxygen often with a combination of steam. Biomass as a product of photosynthesis is one of the most abundant renewable resource that can be used for sustainable production of syngas (a mixture of CO and H₂) [4]. The gasification process requires some gasifying agent that provides oxygen for the formation of CO from solid carbon in the fuel. The gasifying agents include air, oxygen, steam and CO₂ [5]. The gasification process usually begins with drying sub-zone and then followed by pyrolysis. The pyrolysis process leads the breaking down of the biomass into solid matter (charcoal), gaseous mixture (mainly CO₂, CO, CH₄ and H₂) and liquid matter (tar). The main focus in biomass gasification process is to efficiently convert the entire char constituent into gaseous product of the syngas by using either steam or CO₂ [6].

Materials and Methods:

1. Biomass feedstock characterization:

The raw materials used in this study are agricultural residues (coffee bean husk and rice husk) locally produced in Ethiopia's farmlands. These materials were collected from farmlands and local community around Bahir Dar, Ethiopia. The chemistry of biomass gasification is similar to that of coal gasification and the general chemical formula used for the coffee bean husk and the rice husk was CH_{1.76}O_{0.78}N_{0.03} and CH_{1.64}O_{0.95}N_{0.005} respectively. Therefore, stoichiometric air required for complete oxidation of coffee bean husk and rice husk can be calculated from the reaction and 4.58 kg and 4.26 kg of air was required for complete combustion of 1.5 kg of coffee bean husk and rice husk respectively.

2. Proximate Analysis:

A sample of each biomass is taken randomly and tested for proximate analysis to get the comprehensive details of biomass feed. Proximate analysis, which is a standardized procedure that gives an idea of the bulk components that make up a fuel, was done to determine the average of the percentage volatile matter content, percentage ash content, moisture content and percentage content of fixed carbon of the biomass obtained by using ASTM E872, ASTM D1102 and ASTM respectively.[7]

3. Moisture Content (MC):

The percentage moisture content (PMC) was found by weighing of the biomass sample (B₀) and oven drying it at the temperature of 105°C until constant weight of the sample (B₁) was obtained. The loss in weight resulted in the amount of moisture present and sample left in the crucible are total solids present in the sample. The change in weight (B₂) was then used to determine the sample's percentage moisture content by using the following equation:

$$PM=B_2/B_0 \times 100 \quad (1)$$

4. Volatile Matter (VM):

The percentage volatile matter (PVM) was determined by pulverizing the oven dried biomass sample in a crucible and placing it at 550°C for 10 minutes in a Box type resistance furnace Model BK – 5 – 12GJ until a constant weight was obtained and weighed after cooling in desiccators.

The PVM was then calculated by using the following equation

$$PMC = \frac{B_0 - B_1}{B_0} \times 100 \quad (2)$$

5. Ash Content (AC):

The percentage ash content (PAC) was also determined by heating oven dried biomass samples in open silica crucible at 550°C for minimum of 4 hours in Box type resistance furnace Model BK – 5 – 12GJ and weighed after cooling in a desiccator to obtain the weight of ash (C).

$$PAC = \frac{C}{B_0} \times 100 \quad (3)$$

6. Fixed Carbon:

The percentage fixed carbon (PFC) was computed by subtracting the sum of PVM and PAC from 100 as shown in the following equation:

$$\text{Fixed Carbon} = 100 \% - (\text{PAC} + \text{PMC} + \text{PVM}) \quad (4)$$

7. Ultimate Analysis:

This analysis is important for determining the elemental composition (C, N, H, S, O etc.) of the biomass fuels and the empirical formula of biomass as $C_nH_mO_xN_y$ in order to establish stoichiometric equation for complete combustion of biomass and equivalence ratio for the gasification reaction. It was carried out by using EA 1112 Flash CHNS/O- analyzer. For the determination of elemental analysis of the biomass, the following condition was carried out, Carrier gas flow rate of 120 ml/min, reference flow rate 100 ml/min, oxygen flow rate 250 ml/min; furnace temperature of 900 °C and oven temperature of 75 °C.

8. Process Simulation Model Development:

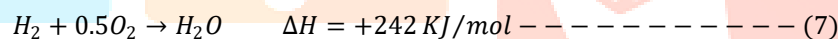
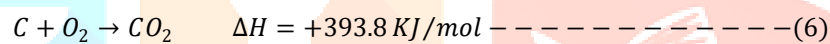
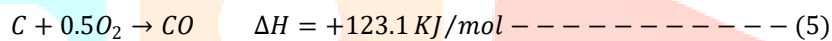
In the area of process modelling and simulation, there are a number of processes modelling software packages available to develop computational model of gasification process and to perform simulation and validation studies. From those types of software packages researchers and professionals use Aspen Plus, Computational Fluid Dynamics (CFD, composed of GAMBIT and FLUENT), Chem-CAD and Mat Lab to develop and optimize the gasification models. From the above mentioned software packages, Aspen Plus is one of the sophisticated processes modeling computer software packages which is familiar to many users and has proven its capacity for gasification model development and simulation [1]. It is a market leading comprehensive chemical process modeling tool, used by the world's leading chemistry organization and related industries. It originated from a joint called Advanced project System for Process Engineering (ASPEN) which is started by the Massachusetts institute of Technology (MIT) and the US Department of engineering in the 1970's and finished in 1981. Aspen Tech was found in the same year and ASPEN project was commercialized Aspen Tech called Aspen Plus[8] Aspen Plus is used in the industrial chemical process modeling,

simulation, optimization, sensitivity analysis and economic evaluation. It provides a comprehensive physical property models and the library of unit operation models, fast and reliable process simulation functions, and advanced calculation method. With the physical property database and the operation models provided by Aspen Plus, engineers are able to simulate actual plant behavior effectively and accurately thereby improve the productivity and reduce the costs.[9]

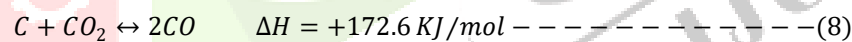
Due to its reliability and precise outcomes in process modeling and simulation, Aspen Plus was used in this study to develop and simulate a fixed bed gasification process for coffee bean husk and rice husk as feed stocks. The simulations process was based on the mass-energy balance and chemical kinetics for the overall process. It comprises several databases containing physical, chemical and thermodynamic data for a wide variety of chemical compounds, as well as a selection of kinetic models required for the accurate simulation of any given system[10]

In Aspen Plus, there is no particular gasifier model ready for use, therefore to model a fixed bed gasifier, it is necessary to separate the whole process into different blocks. The process and the main unit operations involved in the gasification of fixed bed gasifier were drying, pyrolysis (decomposition), gasification and combustion) were simulated by using the reactors RStoic, RYield and RCSTR. As the simulation in this study is based on kinetic modeling, the reaction kinetic parameters are considered. The following assumptions were considered in modeling the gasification process. Process is isothermal and steady state, particles are spherical and are not affected in course of the reaction, the simulation is carried with power-law kinetics, the residence time for reactants is sufficiently high to reach chemical equilibrium and liquid modeling is considered rather than solid modeling for biomass due to unavailability of certain parameters. The gasification reactions which play a great role for the production of syngas from the pyrolysis sub-zone to combustion sub-zone are the following.

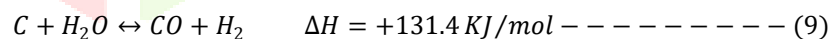
Oxidation reactions:



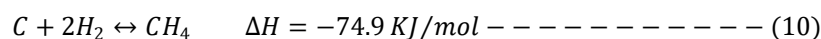
Boudouard reaction:



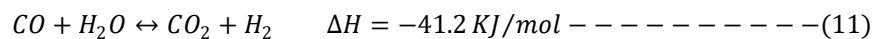
Water gas reaction:



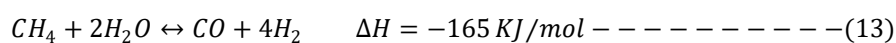
Methanation reaction:



Water gas shift reaction:



Methane reforming reaction:



9. Specifying Components:

In any types of simulation in Aspen Plus after flow sheeting the process specifying the necessary component is important to go the next process. In this fixed bed gasifier simulation process all the components were specified properly. Table 1 lists the components modelled in the simulation. Because the uncertainty of exact formulas of biomass and ash, they were defined as nonconventional solid components. For these components, only enthalpy and density were calculated during the simulation. Aspen Plus includes special models for estimating both enthalpy and density for coal-derived materials. These models can be used to estimate biomass properties as well since biomass can be considered as coal-derived material

Table 1: Detailed data of the components modelled in the simulation [1]

Component ID	Type	Component name	Formula
BIOMASS	Nonconventional	-	-
ASH	Nonconventional	-	-
C	Solid	Carbon-Graphite	C
H ₂	Conventional	Hydrogen	H ₂
N ₂	Conventional	Nitrogen	N ₂
O ₂	Conventional	Oxygen	O ₂
Cl ₂	Conventional	Chlorine	Cl ₂
CO	Conventional	Carbon-Monoxide	CO
CO ₂	Conventional	Carbon-Dioxide	CO ₂
H ₂ O	Conventional	Water	H ₂ O
CH ₄	Conventional	Methane	CH ₄
S	Conventional	Sulfur	S
SO ₂	Conventional	Sulfur-Dioxide	O ₂ S
NH ₃	Conventional	Ammonia	NH ₃
H ₂ S	Conventional	Hydrogen-Sulfide	H ₂ S
HCl	Conventional	Hydrogen-Chloride	HCl

10. Physical Property Method:

For this fixed bed gasifier simulation process, Redlich-Kwong-Soave cubic equation of state with Boston-Mathias alpha function property method was selected as the global property method for this model. It has been used to estimate all physical properties of the conventional components in the gasification process. This property method is comparable to the Peng Robinson cubic equation of state with the Boston-Mathias alpha function (PR-BM) property method. RKS-BM is recommended for gas-processing, refinery and petrochemical applications such as gas plants, crude towers and ethylene plants. This method is generally used for nonpolar or mildly polar mixtures, like hydrocarbons and light gases such as CO₂, hydrogen sulfide and H₂. Using RKS-BM, reasonable results can be expected at all temperatures and pressures. The RKS-BM property method is consistent in the critical region. The enthalpy and density model selected for both feed and ash are non-conventional components, HCOALGEN and DCOALIGT. In this study, feed was defined as non-conventional components and the above model was selected during the simulation process.

11. Specifying Feed stream:

After renaming the stream in the simulation process, it is important to specify all the necessary input streams. In this simulation the biomass (coffee bean husk and rice husk) was specified as non-conventional stream and the ultimate and proximate analyses, given in Table 3.2 were entered. The biomass lower heating value (LHV) was also specified with the HCOALGEN and DCOALIGT property models chosen to estimate the biomass enthalpy of formation, specific heat capacity and density based on the ultimate and proximate analyses. Finally, the stream thermodynamic condition (1bar and 25 °C) and mass flow rate of 1.5kg/hr were used as an input for the process model. The detailed specifications for the inlet streams in this gasification process are listed in table 2.

Table 2: The specifications for the inlet streams in the process model

Stream	Component	Pressure	Temperature	Mass flow rate
BIOMASS	Specified as its proximate, ultimate and sulfur analysis	1bar	25 ⁰ C	1.5 Kg/hr
PRIMARY AIR	21%O ₂ and 79%N ₂ (mole fraction)	1bar	25 ⁰ C	0.3 Kg/hr
SECONDARY AIR	21%O ₂ and 79%N ₂ (mole fraction)	1bar	25 ⁰ C	0.001 Kg/hr

RESULTS AND DISCUSSION:

1. Gasification Temperature:

Gasification temperature is one of the most influential factors affecting the product gas composition and properties. The effect of gasifier temperature on producing syngas composition is shown in figure 1. The temperature considered varies from 400°C to 1400°C when 1.5 kg/hr of the biomass (coffee bean husk and rice husk) and 1 bar of pressure. The concentration of CO is increased with the increase of the gasification temperature while CO₂ concentration followed an opposed manner. The CH₄ concentration is also decreased as the gasification temperature increased. And H₂ is rise with the increasing of gasifier temperature. The temperature of the gasifier is playing a great role in the production of H₂ rich synthesis gas from biomass. As we examine from the following figure the hydrogen gas is increasing with increasing of temperature. These tendencies can be attributed to the chemical reaction laws; the higher temperature favoured the products in endothermic reactions, and favoured the reactants in exothermic reactions.

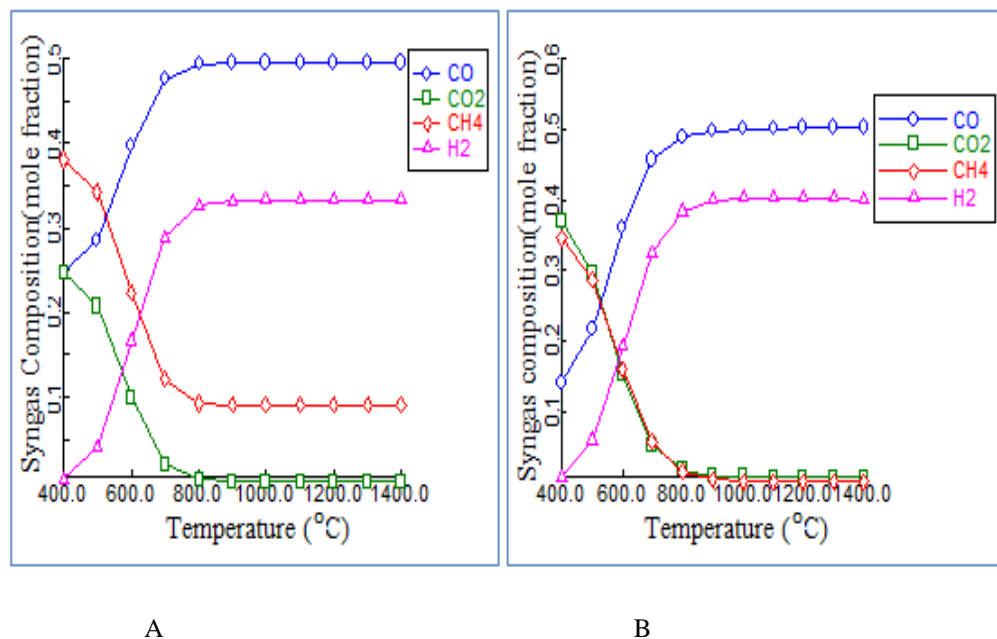


Figure 1: The effect of temperature on the syngas composition (A) for coffee bean husk and (B) for rice husk

2. Gasification pressure:

Pressure is also one of the most gasification factors which influence on the composition of syngas production. The effect of gasifier pressure on produced syngas composition is shown in figure 2. The pressure considered varies from 1 to 10 bars. The result is examined by varying the pressure of the gasifier and making the other parameters kept constant. The amount of the concentration of H₂ and CO is increased at lower pressure in case of the two biomass feed stocks but as the increasing of the gasification pressure the concentration of CO₂ and CH₄ is increased.

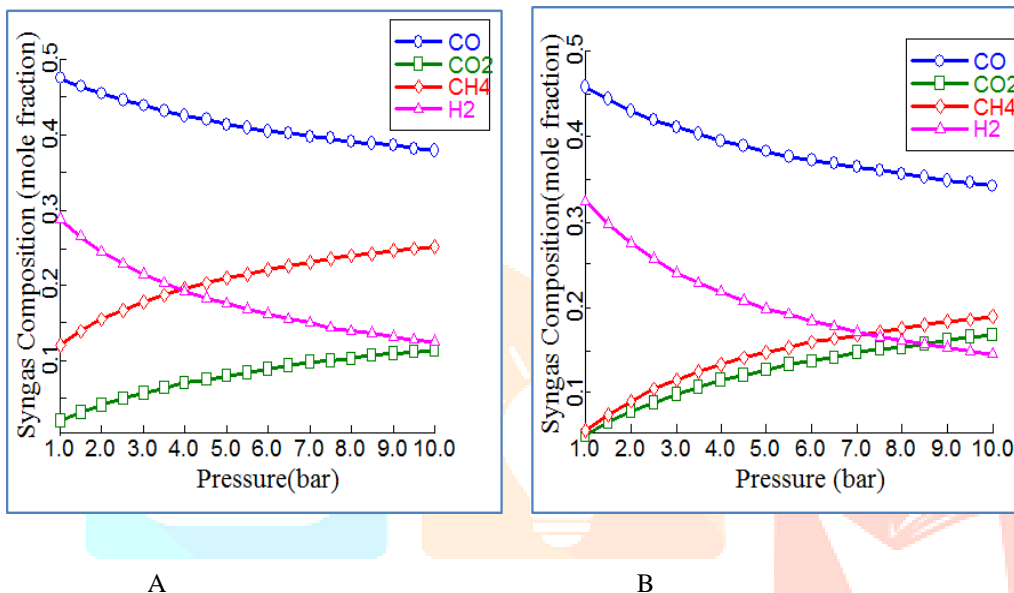
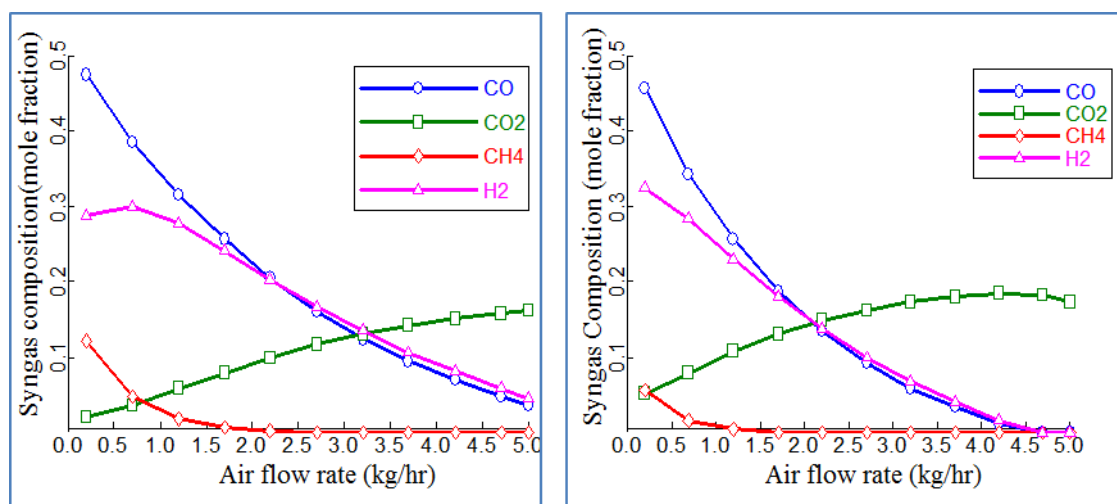


Figure 1: The effect of pressure in the syngas composition (A) for coffee bean husk and (B) for rice husk

3. Equivalence Ratio, ER:

In this gasifier simulation process, the effect of air-biomass ratio on the product gas composition was examined. The simulation results for the syngas composition versus air to biomass ratios covered a range of 0.2 to 1.0 the investigation was made at the value of biomass flow is fixed at 1.5 kg/hr and air mass flow is ranged between 1.67 to 5 kg/hr and the other gasification parameters are unchanged (temperature and pressure). In figure 3 it is obvious that the production of both H₂ and CO decrease with the increasing amount of air. Air to biomass ratio not only represents the O₂ quantity introduced into the gasifier, but also affects the gasification temperature under the condition of auto thermal operation. Higher air to biomass ratios can cause syngas quality to lower because of an increasing oxidation reaction. Alternatively, higher air to biomass ratio means a higher gasification temperature, which can accelerate the gasification and improve the product quality to a certain extent



A

B

Figure 2: The effect of air flow rate on the syngas composition (A) for coffee bean husk and (B) for rice husk

CONCLUSIONS:

In this project, the simulation of biomass gasification for syngas production in a fixed bed reactor was developed using the Aspen plus simulator. The simulation was used to predict the results of biomass gasification, and to provide some process fundamentals about syngas production from the biomass gasification. The effects of gasification temperature, air equivalence ratio and moisture content concentration on the composition of syngas, lower heating value of syngas.

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