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Research Article

Performance Prediction of Gasification of Biomass Briquettes Using Thermodynamic Equilibrium Model

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Abstract

The gasification of biomass resources is considered a promising route for the production of clean energy fuels for the future. The product gas of partial combustion of biomass with air as the gasifying medium is the mixture of CO, H_2, CH_4, CO_2, H_2O and N_2 called syngas. Syngas generation is now considered matured and acceptable technology compared to other biomass conversion technologies. In this study, a thermodynamic equilibrium model to determine syngas composition based on carbon, hydrogen and oxygen obtained from composite agricultural wastes was developed. For these materials, at preset gasification temperature of 750^oC, the effects of changes in moisture content and air/fuel ratio on the quality syngas composition were modeled. The yields of combustible gases (H_2, CO and CH_4) from Rice husk briquette were observed to be generally higher than those of groundnut shell with sawdust briquette. The result with Groundnut shell and Sawdust briquette as input indicated that the fraction of H_2, CO and CH_4 gradually decreased, while the concentration of CO_2 and H_2O increased when moisture content increases from 0% to 45%. Similar trend was observed from the analysis of Rice husk briquette gasification in the model. The amount of Air per kmol of fuel varied from 0 to 1.0. As a result, the H_2, CO and CH_4 content of syngas for Groundnut shell and sawdust briquette decreased continuously; with CH4 approaching zero at air/fuel ratio of unity. Similar trend occurred in Rice husk briquette, but the values were higher than those observed for the groundnut shell & sawdust briquette. The amount of CO_2 and H_2O increased from 14.9742% and 20.6603% to 36.5886% and 57.3208% respectively for Groundnut shell briquette, while for Rice husk briquette the amount of CO_2 and H_2O rose from initial values of 2.8047% and 2.2552% at zero air/fuel ratios to 40.3272% and 45.6339% respectively.

The results of this study would be useful for the engineering development of biomass gasification power generation technologies and in the selection of appropriate feedstock.

Keywords

Gasification—Equilibrium Model—Agricultural waste—Briquette—Moisture Content—Air/fuel ratio.

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Contents

1. INTRODUCTION

Research on and the transition to renewable energy sources is necessitated by global issues such as climate change, environmental sustainability and increasing prices of fossil fuels. The gasification of biomass resources is considered a promising route for the production of clean energy fuels for the future [1, 2]. Gasification can be defined as the conversion of carbonaceous solid or heavy liquid feedstock into product gases with a useable heating value. Commercial gasification processes date back to the late 18th century when coal was converted into town gas for lighting and cooking [3].

Among several kinds of biomass, agricultural residues have become one of the most promising choices. Some agricultural wastes such as wood can be directly utilized as fuels. Nevertheless, a majority of them are not suitable apparently because they are bulky, uneven, and have low energy density. All these characteristics make them difficult to handle, store, transport, and utilize in their raw form. Hence, there is the need to subject them to conversion processes in order to mitigate these problems. One of the promising solutions to these problems is the application of briquetting technology [4]. Briquettes are compacted combustible material that are created from biomass residue, charcoal dust or coal dust and are used as a form of fuel for heating or cooking. These are products of the densification process, which is a two-part process that involves compaction (reduction in volume) and binding (ensuring the product remains in the compacted state)[5].

For a techno-economical evaluation, actual construction of a gasifier is not always feasible and economically sound because experimentation usually involves much greater time, effort, and cost. Thus, a mathematical model for such analysis is more useful [6]. The gasification process has been studied from the theoretical point of view, and different mathematical models have been built to try to simulate the thermochemical processes and to evaluate the influence of the main parameters such us temperature, moisture content, air/fuel ratio, steam/fuel ratio, gas composition and its heating value. Some models only look for the final gas composition at chemical equilibrium, while others try to reproduce the different sub processes along the reactor. The models can be divided in three groups: equilibrium models (stoichiometric and non-stoichiometric), kinetic models and neural network models. Models where both equilibrium and kinetic aspects are linked have been also developed [7]. The thermodynamics equilibrium model is simplest and provides the output with reasonable accuracy [8].

The equilibrium model (based on the minimization of Gibbs free energy or based on equilibrium constant) has been used by many researchers for the analysis of the gasification process. Zainal et al. [9] used the latter type of equilibrium model to predict the composition of the producer gas for different biomass materials. The Gibbs free energy minimization method was used by a group of researchers (S. Jarungthammachote and A. Dutta) to predict the composition of the producer gas in spouted bed gasifier. The major six components, CO, H_2, CH_4, CO_2, H_2O and N_2 were determined in the mixture of the producer gas. The results showed that the carbon conversion in the gasification process plays an important role in the model. Thermodynamic model based on the minimization of Gibbs free energy was simulated by S. Pandey et al. to study the effect of preset reaction temperature with respect to moisture content on gas mole fraction at the output of the downdraft gasifier. Equivalence ratio and output gas higher heating values variation of the downdraft gasifier are also predicted for various values of moisture content. In this work, a thermodynamic equilibrium model focusing on gasification of two briquettes of composite agricultural waste from risk husk, and groundnut shell & sawdust was developed. For these materials, at preset gasification temperature, the influence different moisture contents have on the quality syngas produced is modeled. The effects of air/fuel ratio on syngas composition are also investigated. The model best predicts the syngas composition when the reaction temperature is sufficiently high and it is more accurate to compare the results with downdraft gasifier type as it is the only gasifier that exits with lower tar concentration [9].

2. MATERIAL AND METHODS

2.1 ASSUMPTIONS

In this study, the formulation of the thermodynamic model was based on the following assumptions:

- All carbon content in biomass is converted into gaseous form and the residence time is high enough to achieve thermodynamic equilibrium.
- All the gaseous products are assumed to behave as ideal gases.
- The amount of tar in syngas was assumed to be negligible.
- The reaction was auto-thermal and no external source of heat was applied.
- Ash in the feedstock was assumed inert in all gasification reactions although it holds true typically only for reaction temperatures less than 700^{o}C

2.2 MODEL FORMULATION

The chemical composition of biomass is taken to be in the form CHxOyNz and the gasification reaction can be written in the following form:

$$CHxOyNz + wH_2O + x_g(O_2 + 3.76N_2) \rightarrow x_1CO + x_2H_2 + x_3CO_2 + x_4H_2O + x_5CH_4 + (z/2 + 3.76x_g)N_2 \quad (1)$$

Where x, y and z are the number of atoms of hydrogen, oxygen and nitrogen per number of atom of carbon in the feedstock respectively. w and x_g are the amount of moisture and air per kmol of feedstock respectively. All input in the left hand side of equation 1 is defined at 25oC. On the right hand side, x_i (i=1, 2, 3, 4, 5) are the numbers of mole of the species i that are also unknown.

w can be calculated using the following relation:

$$w = \frac{M_{biomass} \times M_{moist}}{18[1 - M_{moist}]} \quad (2)$$

Where $M_{biomass}$ is the molar mass of biomass feedstock and M_{moist} is moisture content of feedstock.

To find the five unknown species of the producer gas, five equations are required. These equations are generated using mass balance and equilibrium constant relations of combined biomass gasification equation. From equation 1, taking atom balances on carbon, hydrogen and oxygen, the first three equations are formulated as shown.

$$X_1 + X_3 + X_5 = 1 \quad (3)$$

$$x + 2w = 2x_2 + 2x_4 + 4x_5 \quad (4)$$

$$y + w + 2x_g = x_1 + 2x_3 + x_4 \quad (5)$$

The remaining two equations are obtained from the equilibrium constant of the major reactions that occur inside the reactor.

$$C + CO_2 \rightarrow 2CO \quad (6)$$
$$C + H_2O \rightarrow CO + H_2 \quad (7)$$

Equations 6 and 7 are the Boudouard reaction and water-gas reaction respectively. The two reactions can be combined into one single reaction known as water-gas shift reaction.

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (8)$$

The other prominent reaction in the gasification process is methanization reaction.

$$C + 2H_2 \rightarrow CH_4 \quad (9)$$

The equilibrium constant for these two equations 8-9 as the function of their molar mass composition can be written as:

Stoichiometric equilibrium constant for water-gas shift reaction:

$$k_1 = \Pi_i (x_i)^{v_i} (\frac{p}{p_o}) \Sigma_i v_i = \frac{p_{CO_2} p_{H_2}}{p_{CO} p_{H_2O}} = \frac{n_{CO_2} n_{H_2}}{n_{CO} n_{H_2O}} = \frac{x_3 x_2}{x_1 x_4} \quad (10)$$

Equilibrium constant for methane reaction:

$$k_1 = \Pi_i (x_i)^{v_i} (\frac{p}{p_o}) \Sigma_i v_i = \frac{p_{Ch_4}}{p^2_{H_2}} = \frac{n_{Ch_4} n_{total}}{n^2_{H_2}} = \frac{x_3 x_{total}}{x_2{}^2} \quad (11)$$

Where x_i is mole fraction of species in the ideal gas mixture; v is stoichiometric number; po is standard pressure, 1 atm; ntotal is total mole of producer gas.

Equations 3.10 and 3.11 can be modified as

$$K_1(x_1 x_4) = x_2 x_3 \quad (12)$$
$$K_2(x_2^2) = x_5 x_{total} \quad (13)$$

The equilibrium constants in Equations 12-13 are obtained from Equation 14.

$$\ln k(T) = \frac{-\Delta G_T}{RT} \quad (14)$$
$$\Delta G_T = \sum_i x_i \Delta g_{f,T,i} \quad (15)$$

Where $\Delta g_{f,T,i}$ is empirically derived according to the equation

$$\Delta g_{f^o,T,i} = H_{f^o,i} - aT\ln T - b\ln T^2 - \frac{c}{2}T^2 - \frac{d}{3}T^4 + \frac{e}{2T} + f + gT \quad (16)$$

The values of a-g in Table 1 below are taken from Probstein and Hicks along with enthalpy of formation at standard reference state of 298 K (250C) and 1 atm pressure [10]. R is the universal gas constant, 8.314kJ/kmol.K. ΔG_T is the standard Gibbs function of reaction and $\Delta g_{f^o,T,i}$ represents the standard Gibbs function of formation at given temperature T of gas species i.

Table 1. Standard heat of formation, and empirical coefficients for Equation 16 [10]

Species		a	b	c	d	e	f	g
CH4	-74.8	-4.62x10-2	1.13x10-5	1.32x10-8	-6.65x10-12	-4.89x10-2	14.1	-0.223
CO	-110.5	5.62x10-3	-1.19x10-5	6.38x10-9	-1.85x10-12	-4.89x10-2	0.868	-0.0613
CO2	-393.5	-1.95x10-2	3.12x10-5	-2.45x10-8	6.95x10-12	-4.89x10-2	5.27	-0.121
H2O	-241.8	-8.95x10-3	-3.67x10-6	5.21x10-9	-1.48x10-12	0	2.87	-0.0172

To solve for all unknown, the only the energy balance equation is required. The enthalpy of reactants entering must be the same as the enthalpy of product leaving the system.

$$\sum_j H_{f,j,reactant} = H_{f^o,biomass} + \sum_{j=m_w,x_g} n_i (H_{f^o,i} + \Delta H_{T^o,i}) \quad (17)$$

$$\sum_j H_{f,j,reactant} = \left(\frac{z}{2}\right) + 3.76 x_g \Delta_(298 - Tout) h_(T, N_2) + \sum_i^5 n_i (\Delta_{298-Tout} h_{T,i} + h_{f^o,i}) \quad (18)$$

h_f^o is the enthalpy of formation in kJ/kmol and its value is zero for all chemical element at reference state (298k, 1atm).

$$\Delta h_f^o = \int_2 98^T C_p(T) dT \quad (19)$$

where $C_p(T)$ is specific heat at constant pressure in kJ/kmol.K. The heat of formation for biomass can be calculated from the model developed by Zainal et.al [10].

$$H_{f^o,biomass} = LHV \quad (20)$$

LHV is calculated in dry basis of biomass and is calculated using the following equation:

$$LHV = 4.187(18C + 300H - 26(O-S) - 6(9H+m)\left(\frac{kJ}{kg}\right) \quad (21)$$

The total enthalpy content can be written as follows:

$$H_{f^o-biomas} + m_w(H_{f^o_{H_2O(l)}} + H_{vap}) + x_g(H_{f^o_{O_2}} + 3.76H_{f^o_{N_2}}) = x_1(H_{f^o_{C}O} + \int_2 98^{T_g} C_{p_{CO}} dT) + x_2(H_{f^o_{H_2}} + \int_2 98^{T_g} C_{p_{H_2}} dT) + x_3(H_{f^o_{CO_2}} + \int_2 98^{T_g} C_{p_{CO_2}} dT) + x_4(H_{f^o_{H_2O}} + \int_2 98^{T_g} C_{p_{H_2O}} dT) + x_5(H_{f^o_{CH_4}} + \int_2 98^{T_g} C_{p_{CH_4}} dT) + \left[(\frac{z}{2} + 3.76x_g)\int_2 98^{T_g} C_{p_{N_2}} dT\right] \quad (22)$$

This equation acts as the constraint for the gasification process and forms the basis for adjusting the amount of air to be supplied.

Cp can be determined using empirical relation that holds for a wide range of temperature,

$$C_p(T) = C_1 + C_2T + C_3T^2 + C_4T^3 \left(\frac{kJ}{kg}\right) \quad (23)$$

The sensible heat of each gas species can be found by integrating equation (3.23) from the ambient temperature to the gasification temperature.

$$\int_2 98^T C_p(T)dT = C_1T + \frac{C_2}{2}T^2 + \frac{C_3}{3}T^3 + \frac{C_4}{4}T^4 \left(\frac{kJ}{kg}\right) \quad (24)$$

Values of C_1, C_2, C_3 and C_4 are got from Desta, 2011 [11].

The system of equations above solve for the values of nH_2; nCO; nCO_2; nH_2O and nCH_4. An initial temperature of 750^oC was assumed and substituted into Equations (14) and (16) to initially calculate K1 and K2. Then, both equilibrium constants were substituted into Equations (12) and (13), respectively. The five simultaneous equations, Equations (3.3, 3.4, 3.5, 3.8, and 3.9) are solved using symbolic function in MATLAB. The model was run with elemental compositions of the biomass briquettes.

3. RESULTS AND DISCUSSION

The equilibrium model described is used for the gasification of briquettes. Typical results obtained are presented for two composite agricultural wastes for comparison because biomass elemental composition has significant effect on syngas composition. The release of pyrolysis gas is highly dependent on hydrogen/carbon ratio as well as oxygen/carbon ratio and increases when these ratios increase, especially with an increase in Hydrogen/Carbon ratio. A higher oxygen concentration in biomass needs lower Equivalence ratio for gasification because of its inherent oxygen that will also be available for gasification.

3.1 Ultimate Analysis

The ultimate analysis of the composite agricultural wastes is presented in Table 2. By substituting the values of C, H, O, N, and S into the model, the yield and composition of briquettes gasification were deduced.

Table 2. Ultimate Analysis of Composite Agricultural Waste

Parameter	Unit	Briquette	
		Groundnut Shell & Sawdust [12]	Rice Husk [13]
Carbon (C)	%	53.1	42.1
Hydrogen (H)	%	8.1	5.8
Oxygen (O)	%	35.75	51.67
Nitrogen (N)	%	0.02	0.05
Sulfur (S)	%	0.93	0.38

3.2 Model Validation

In order to validate the results from the equilibrium model developed for this study, experimental data taken from the literature were used and compared to the results predicted by the model. The results are shown in Figure 1.

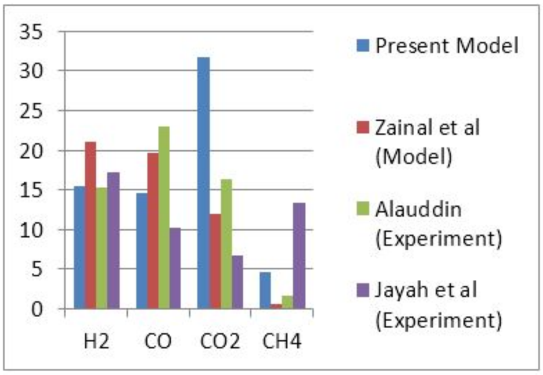

Figure 1. Comparison of Present model with experimental results and a model by Zainal et al.

3.3 Effect of Moisture Content on Syngas Composition

Moisture content is an important parameter for biomass briquettes and it depends on many factors such as the mechanism of production mechanism, storing and transportation conditions. Therefore, analyzing the effect of moisture content on producer gas composition and gasification characteristics is of great importance. The effects of moisture content on the producer gas composition for the two briquettes under consideration are shown in Figure 2 and 3.

As can be observed from Figure 2 below, an increase in moisture content from 0% to 45% leads to almost a linear decrease (from 26.2728% to 18.6007%) in the composition of H_2 and (from 19.9497% to 6.5164%) in CO. The composition of Methane (CH_4) dropped slightly from 13.6496% to 10.3624%. CO_2 remained relatively constant while H_2O increased from 22.8075% to 47.7797% with increase in moisture content.

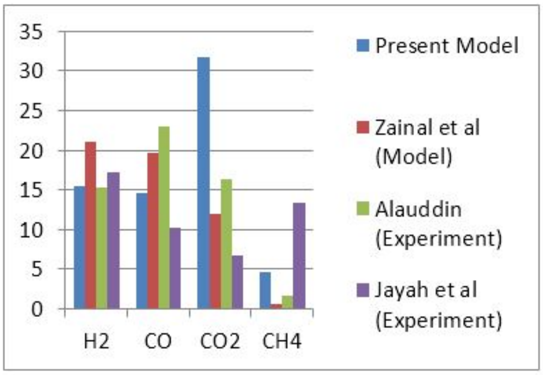

Figure 2. Effect of Moisture Content on Syngas Composition for Groundnut Shell & Sawdust Briquette

For the Rice husk briquette, it can be observed from Figure 3 that the combustible constituents (H_2, CH_4 and CO) are of higher values than the values from briquette of Groundnut + Sawdust. These values also dropped with increase in moisture content as expected.

In order to produce syngas from biomass, the moisture content should be less than 20%; otherwise, the bio-mass should be dried before entering the gasifier.

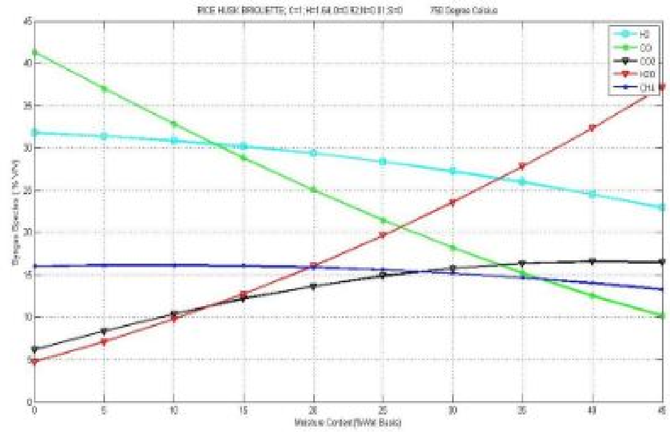

Figure 3. Effect of Moisture Content on Syngas Composition for Rice Husk Briquette

3.4 Effect of Air/fuel ratio on Syngas Composition

The influence of air supplied on gasifier performance is illustrated in figures 5 and 6. Air/fuel ratio was varied from 0 to 1.0 kg per kmol of feedstock. As a result, the H_2, CO and CH_4 content of syngas for Groundnut shell + sawdust briquette decreased continuously, with CH4 approaching zero at air/fuel ratio of unity (Figure 4). The amount of CO_2 and H_2O increased from 14.9742% and 20.6603% to 36.5886% and 57.3208% respectively.

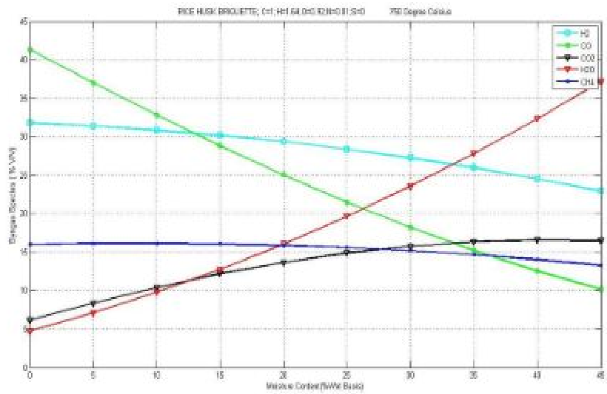

Figure 4. Effect of Air/fuel ratio on syngas Composition for Groundnut shell & sawdust Briquette

Changes observed in the values of constituent gases for the Rice husk briquette were due to the elemental composition (Figure 5). The amount of CO_2 and H_2O rose from initial values of 2.8047% and 2.2552% at zero air ratios to 40.3272% and 45.6339% respectively. Values of the combustible components were higher than those observed for the groundnut shell & sawdust briquette. A similar trend in the composition of H_2, CO and CH_4 was also observed like in the groundnut shell & sawdust briquette, however, the decreased was from 34.1111% to 6.9146%, 42.4172% to 6.1098% and 18.4118% to 1.0145% respectively, as the ratio of air to fuel approached unity.

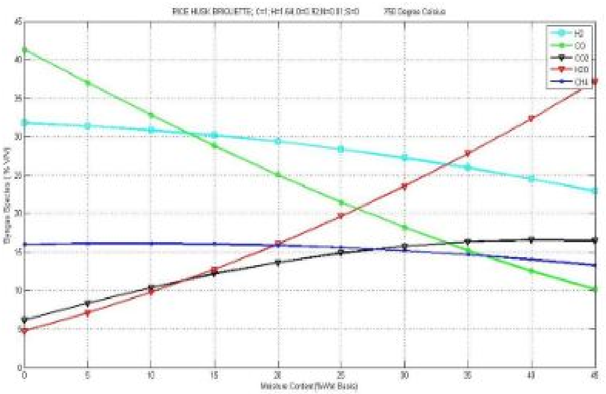

Figure 5. Effect of Air/fuel ratio on syngas Composition for Rice husk briquette

3.5 CONCLUSION

A thermochemical equilibrium model was developed for gasification of Rice husk and Groundnut + Sawdust briquettes in order to calculate the composition of the producer gas and investigate the gasification characteristics. The predicted results agreed reasonably with those of the experiments available in the literature. The effects of moisture content and air/fuel ratio on gasification characteristics were investigated.

Hence, it can be concluded that the thermodynamic equilibrium model developed in this study is robust, flexible and can be used to simulate gasification of other types of biomass materials and to predict the effect of other important variables in the optimization of biomass downdraft gasifier.

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