

On a Numerical Model for Gasification of Biomass Materials

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Abstract: In this paper, a thermochemical equilibrium model is used to predict the performance of a downdraft gasifier. Numerical results are shown to be in good agreement with those of the experiments. Different biomass materials are tested using the model and forest residual is shown to be the most energetic one. For this material, the gasification temperature, syngas composition and calorific value are calculated. The effects of moisture content, air/fuel ratio, air inlet temperature and steam/fuel ratio are also investigated. The air inlet temperature is found to be the only way to increase the gas calorific value and cold gas efficiency. The steam/fuel ratio, on the other hand, plays a key rule in controlling the gasification temperature and H₂/CO ratio.

Keywords: Renewable Energy, Biomass, Gasification, Thermochemical Equilibrium, Mathematical Modeling

1 Introduction

Biomass as a new source of energy has drawn world wide attention during the last decade. Positive rate of consumption of fossil fuels, negative rate of their natural reservoirs and restricting environmental rules have created awareness for the need to identify alternative sources of fuel such as biomass. Byproducts of activities like agriculture or food processing are categorized as biomass materials. These materials were used to dispose in open lands creating serious environmental problems. Composting, recycling and incineration have been used as alternative methods for waste handling [1]. More recently, gasification of biomass materials has been introduced as another kind of waste to energy (WTE) conversion; a process to convert carbonaceous materials to synthetic gases such as CH₄, CO, CO₂ and H₂. One of attractive features of this technology include the ability to produce a clean syngas product that can be used either for generating electricity or producing chemicals.

It must be understood that gasification is *not* combustion. A combustion process needs stoichiometric feed of air/oxygen, while gasification process is performed at sub-stoichiometric conditions (30% to 70% of stoichiometric air/oxygen). In some cases, nitrogen and/or steam are also injected in order to control the gasification condition and volume of products. The many advantages of gasification over combustion make it feasible to review the possibilities of syngas production as a sink for biomass materials while

observing the environmental regulations. In this technology, solid feed materials are gasified in a reactor such that virtually all of their contents are converted into fuel gas with calorific values typically 3±6 MJ/m³ (natural gas is 34 MJ/m³) with most of the energy being available from H₂ and CO. After cleaning, this gas can be used to run small reciprocating engines, boilers, process heaters etc. Biomass gasification is a complex process with many important controlling parameters such as air/fuel ratio and moisture content. As a result, mathematical models have been introduced for predicting the performance of gasifiers and as tools for their design optimization [2–4]. One of these models, the equilibrium modeling, was used by many researchers. Although, thermodynamic equilibrium in reality never takes place in a gasification process [5], several works were performed to demonstrate the applicability of the equilibrium model for this process. These models especially work well in high temperatures that occur in entrained flow gasifiers (above 1500K) [6]. Some equilibrium models were based on the minimization of Gibbs free energy [7-8] while others were based on equilibrium constant.

Altafini and Mirandola [4] simulated a biomass gasifier, based on minimizing the Gibbs free energy. The biomass gasification process was also modeled by Zainal et al. [9] based on equilibrium constants. Lapuerta et al. [10] predicted the producer gas composition as a function of the fuel/ air ratio by means of an equilibrium model. A description of a

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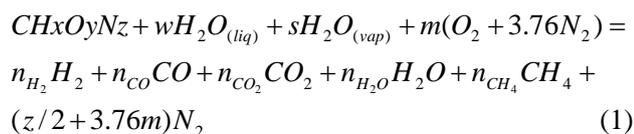
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two-zone model in a downdraft gasifier was adapted by Jayah et al. [7] and Schuster et al. [11]. An experimental study was also described by Zainal et al. [12].

A zero-dimensional model presented in this paper is based on the thermochemical equilibrium of the process using equilibrium constants. Numerical model is first validated by a comparison between calculated results and two separate experiments available in the literature [2-4]. The effect of ultimate analysis on the calorific value is studied for 20 different common biomass materials and the most energetic one is selected as a sample for rest of the paper. The influence of important parameters of a gasification process such as: the air/fuel ratio, biomass moisture content, air preheating, and steam injection on the gasification characteristics are also investigated. These characteristics are the syngas composition, gasification temperature, calorific value of the producer gas and the cold gas efficiency.

2 Methodology

The main assumptions of the developed model are as follows. The gasifier reactor is assumed to be adiabatic and the residence time of the reactants is supposed to be high enough to reach chemical equilibrium. In addition, all carbon in the biomass is assumed to be gasified and, therefore, the formation of char is neglected. To develop the model, the chemical formula of feedstock is defined as $CH_xO_yN_z$. The global gasification reaction can be written as follows:



where x , y , and z are numbers of atoms of hydrogen, oxygen, and nitrogen per one atom of carbon in the feedstock; respectively, and w , m , and s are the amounts of moisture, air, and steam per one kmol of feedstock, respectively. All inputs on the left-hand side of Eq.(1) are defined at $25^\circ C$. On the right-hand side, n_i is the number of moles of the species i which is also unknown. Molar quantity of water per one kmol of biomass can be written as [9]:

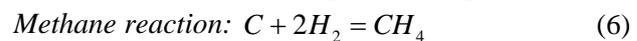
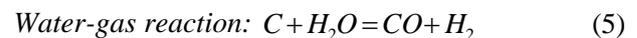
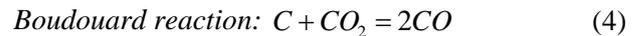
$$w = \frac{M_{bm} \times MC}{M_{H_2O} \times (1 - MC)} \quad (2)$$

where M_{bm} and M_{H_2O} are the masses of the biomass and water; respectively, and MC is the moisture content. Air/fuel ratio can be calculated

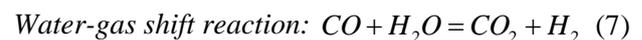
as $(\alpha + 0.25\beta - 0.5\gamma)$ for a fuel with a chemical formula of $C_\alpha H_\beta O_\gamma N_\xi$ [13]. During the gasification process, only between 30% and 70% of stoichiometric air is used; therefore, we assume m to be a fraction of the calculated stoichiometric air. In addition, the enthalpy of formation for biomass can be obtained as follows [14]:

$$h_{f,bm}^\circ = LHV_{db} + \frac{1}{M_{bm}} \sum_{i=prod} v_i h_{f,i}^\circ \quad (3)$$

where h_f° is the enthalpy of formation, LHV is the lower heating value and v_i is the stoichiometric coefficient of the species i . To obtain the five unknown species of the producer gas, five equations are required which are generated using mass balance and equilibrium constant relationships. Considering the global gasification reaction in Eq.(1), the first three equations are formulated by balancing each chemical element consisting of carbon, hydrogen and oxygen. The remaining two equations are obtained from the equilibrium constant of the reactions that occur in the gasification zone which are given as:



Higman and van der Burgt [15] showed that Eqs.(4) and (5) can be combined to give the water-gas shift reaction as:



For the model in this study, in addition to an assumption of thermodynamic equilibrium, all gases are assumed to be ideal and all reactions to occur at the atmospheric pressure. Therefore, the equilibrium constants, which are functions of temperature, for the methane and the water-gas shift reactions can be written based on the following:

$$K = \prod_i (x_i)^{v_i} \left(\frac{P^\circ}{n_{total}} \right)^{\sum_i v_i} \quad (8)$$

where x_i is mole fraction of the species i in the ideal gas mixture, v is the stoichiometric number, P° is the standard pressure (1atm) and n_{total} is the total number of moles of product gas. As a result, the equilibrium constants for the water-gas shift and the methane reactions will be as follows:

$$k_1 = \frac{(n_{CO_2})(n_{H_2})}{(n_{CO})(n_{H_2O})} \quad (9)$$

$$k_2 = \frac{(n_{CH_4})}{(n_{H_2})^2} \quad (10)$$

The values of the equilibrium constants, which are mere functions of temperature, can be calculated using the Gibbs free energy:

$$\ln k = \frac{-\Delta G_T^\circ}{\tilde{R}T} \quad (11)$$

where \tilde{R} is the universal gas constant and ΔG_T° is the standard Gibbs function of formation. The dependence of ΔG° on temperature can be written as follows:

$$\frac{d(\Delta G^\circ / RT)}{dT} = \frac{-h_f^\circ}{\tilde{R}T^2} \quad (12)$$

where h_f° is the enthalpy of formation with a value of zero for all chemical elements in a reference state. Therefore, based on Eq.(11) we will have:

$$\frac{d \ln k}{dT} = \frac{h_f^\circ}{\tilde{R}T^2} \quad (13)$$

Since the heat of formation is a function of T, Eq.(13) can be integrated as follows:

$$\ln k = \int \frac{h_f^\circ}{\tilde{R}T^2} dt + I \quad (14)$$

The amounts of ΔG° and h_f° can be found in chemical engineering handbooks [17].

Jarunthammachote et al. [16] multiplied k_2 [see Eq. (10)] by a factor to improve the performance of the model. The same factor is used in this model. The temperature of the gasification zone needs to be determined in order to calculate the equilibrium constants [Eq.(11)]. For this reason, a balance of either energy or enthalpy is performed on the gasification process usually assumed to be adiabatic. If the temperature in the gasification zone is T and that of the inlet state is assumed to be 298K, the enthalpy balance for this process can be written as:

$$\sum_{j=react} n_j h_{f,j}^\circ = \sum_{i=prod} n_i (h_{f,i}^\circ + \Delta h_{T,i}^\circ) \quad (15)$$

where Δh_T° represents the enthalpy difference between any given state and the reference state. It can be approximated by:

$$\Delta h_T^\circ = \int_{298}^T \bar{C}_p(T) dT \quad (16)$$

where $\bar{C}_p(T)$ is the specific heat at constant pressure which is only a function of temperature. It is defined by an empirical relation as [17]:

$$\bar{C}_p(T) = C_1 + C_2 \left[\frac{C_3}{\sinh\left(\frac{C_3}{T}\right)} \right]^2 + C_4 \left[\frac{C_5}{\sinh\left(\frac{C_5}{T}\right)} \right]^2 \quad (17)$$

When the equilibrium constants are defined, a system of equations will be obtained that need to be solved. Because of the non-linear nature of some of the equations, the Newton–Raphson method is used which can be solved with an iterative procedure. The procedure starts with an initial guess for the gasification temperature. The set of equations are then solved to obtain the producer gas composition which in turn is used to determine the new gasification temperature [using Eq. (14)]. This iterative procedure continues until the gasification temperature does not change within a certain limit (much less 1 K) in successive iterations.

3 Results and discussion

In this section, the results of the presented model for producer gas composition are first compared to those of the experiments performed by Jayah et al. [2] and Altafini et al. [4] as shown in Table 1. Jayah et al. [2] calibrated their model by the methane content. In this model, the thermal losses in the gasifier were not taken into account; therefore, the predicted values for methane are slightly less than those of the experiments. The slight differences in other components (seen in Table 1) may be attributed to the simplifying assumptions of the model such as: considering all gases to be ideal, and assuming no char or residue in the gasification process. As seen from the table, the thermochemical equilibrium model can predict the measured values with a high accuracy ($RMS < 2$).

Table 1 The comparison of experimental data [2,4] with the predicted results

	Reference [2] ^a		Reference [4] ^b	
	Exp	Model	Exp	Model
H ₂	17.2	15.8	14.0	15.2
CO	19.6	20.0	20.1	22.3
CO ₂	9.9	11.4	12.0	9.8
CH ₄	1.4	0.7	2.31	0.59
N ₂	51.9	51.9	50.7	51.8
CV MJ/m ³	---	4.82	5.27	5.01
RMS ^c error	0.998		1.56	

^a Rubber Wood -18.5% moisture content

^b Sawdust -10% moisture content

$$RMS = \sqrt{\frac{\sum_i^N (Exp_i - Num_i)^2}{D}}$$

In order to compare various biomass sources of energy, gasification of 20 different samples are simulated under the same conditions (biomass with zero moisture content and stoichiometric coefficient equal to 0.46) to evaluate their producer gas calorific values. These samples were selected across five major groups of biomass materials [18] consisting of grasses and straws; wood fuels; urban waste fuels; wood fuel blends; nuts, pits and shells. The results of the simulations for the twenty samples are shown in Fig. 1. As seen from the figure, forest residuals are found to produce the highest calorific value (4.73 MJ/m³). Ultimate analysis of this biomass (forest residual) is 50.31%*C*, 4.59%*H*, 39.99%*O*, 1.03%*N*, 0.11%*S* and a *HHV* of equal to 459.61 MJ/kmol.

An important parameter for a biomass material is its moisture content which depends on many factors such as the production mechanism, and storing and transportation conditions. Therefore, analyzing the effect of moisture content on producer gas composition and gasification characteristics is of great importance. The effect of moisture content on the producer gas composition is shown in Fig.2. As observed, an increase in moisture content from 0% to 40% leads to a 31.8% increase of H₂ and 89.8% of CO₂, but a 42.69% decrease of CO. The effect of moisture content on calorific value and gasification temperature is shown in Fig.3. It can be seen from

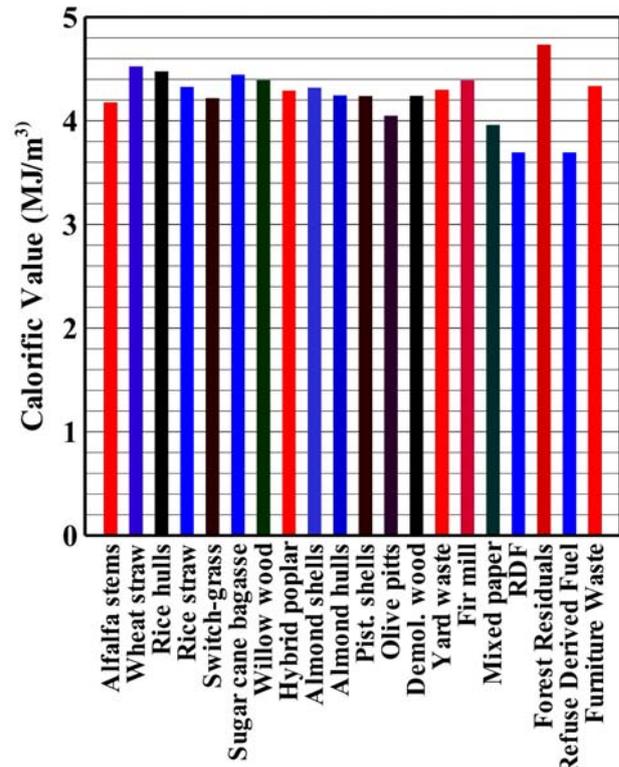


Figure.1 Comparison between calorific values obtained via gasification of 20 different biomass materials

the figure that increasing the moisture content reduces the calorific value of the producer gas. Although the calorific values of H₂ and CO (energetic gases) are close to each other (241.8 MJ/kmol and 282.9 MJ/kmol), since the decrease of CO is greater than the increase of H₂, the resultant calorific value of the producer gas is decreased. Figure 3 also shows that increasing the moisture content reduces the gasification temperature. This is because a greater moisture content means more required energy for vaporization. The above results are in good agreement with the numerical results of Zainal et al. [9] and Jarunthammachote et al. [16]. To investigate other parameters, the effect of air inlet temperature is also studied. It was found that air preheating can increase the calorific value of the producer gas. For an increase of air temperature from 300K to 600K, the producer gas composition was not changed considerably; however, the calorific value was increased by 0.6% and the

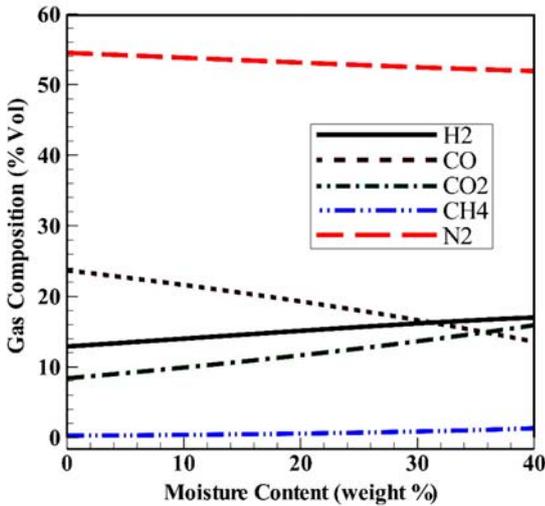


Figure.2 Effect of moisture content on gas composition

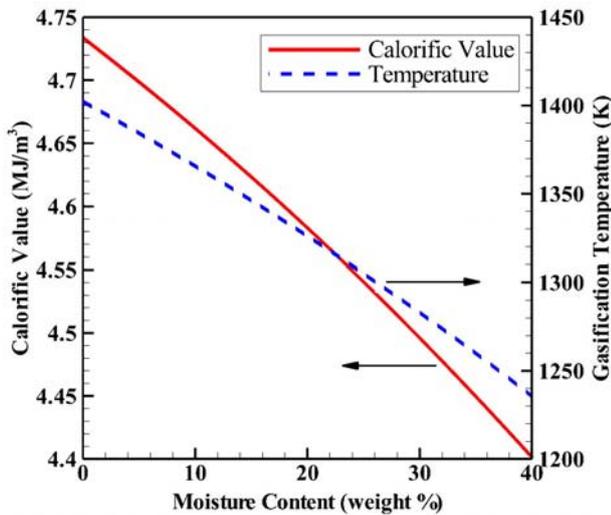


Figure.3 Effect of moisture content on gasification temperature and calorific value of the producer gas
 gasification temperature by 130K. The slight increase of calorific value (only 0.6%) does not justify the increase of the air inlet temperature because of the considerable increase of the gasification temperature (by 130K) which is not favored.

Gas composition variations against air/fuel ratio are plotted in Fig.4. As it was discussed before, the air/oxygen stream of a gasification process should be between 30% to 70% of the stoichiometric air/oxygen. If this portion is increased, the process nears the usual combustion with a tendency to produce CO₂ and N₂ (dominant products of combustion process). This will increase the temperature and considerably decrease the calorific value of the producer gas.

The effect of steam/fuel ratio on calorific value of the producer gas and the gasification temperature is shown in Fig. 5. Steam in gasification is called "moderator" because it can be used as a means for controlling the gasification temperature (see Fig. 5).

In addition, it can be used to adjust H₂/CO ratio and increase the volume of CH₄ in the producer gas. Finally, we study the influence of four effective parameters on cold gas efficiency (also known as the first law of thermodynamics efficiency) defined as the ratio of the energy leaving the gasifier to the energy entering it (i.e. biomass and moisture). Evaluating the energy of the producer gas and that of the feedstock in the same state (reference temperature), the cold gas efficiency is written as:

$$CGE = \frac{\text{Heating value in producer gas (MJ)}}{\text{Heating value in feed stock (MJ)}} \quad (18)$$

Figure 6 shows the results of the model for the effect of important parameters on CGE. While increasing the air inlet temperature causes a slight increase of

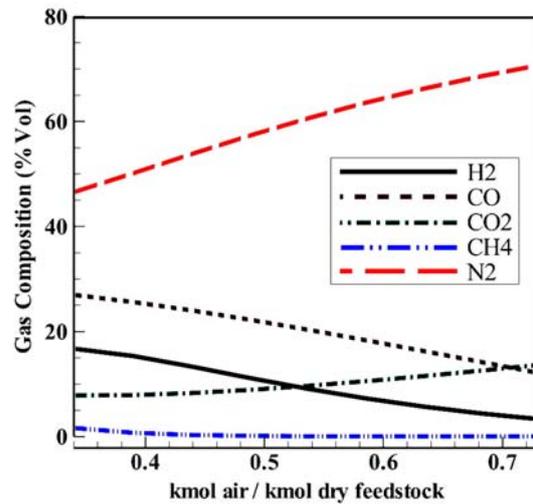


Figure.4 Effect of air/fuel ratio on gas composition
 cold gas efficiency, other parameters have a reverse effect.

4 Conclusion

A thermochemical equilibrium model was developed for a biomass gasifier in order to calculate the composition of the producer gas and investigate the gasification characteristics. The predicted results agreed well with those of the experiments available in the literature. The model

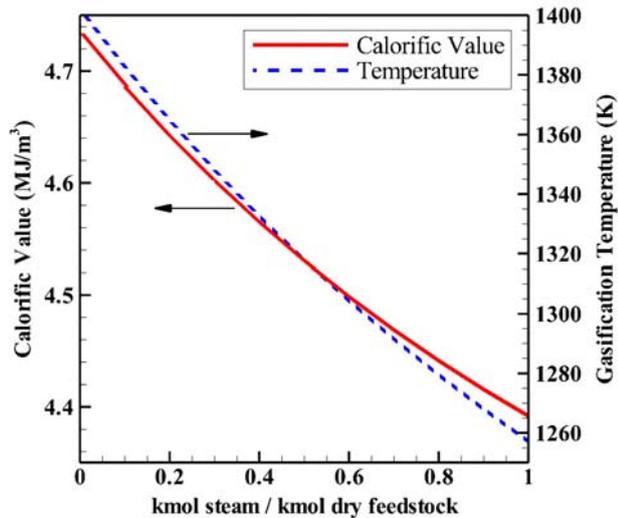


Figure.5 Effect of steam/fuel ratio on calorific value of the producer gas and gasification temperature

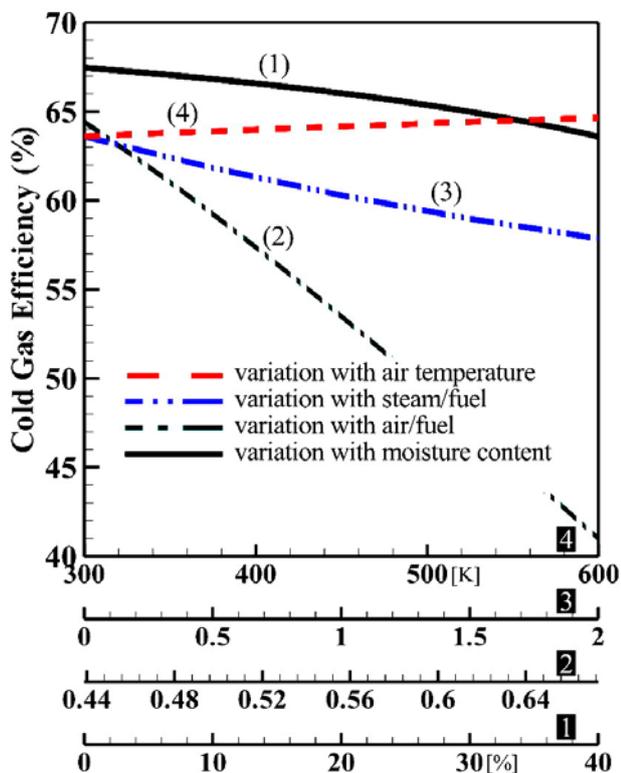


Figure.6 Influence of four effective parameters on cold gas efficiency

was then employed to evaluate the capability of different biomass materials to produce energy. Among twenty different biomass materials of five major families, forest residuals had the highest calorific value. The effects of moisture content, air inlet temperature, air/fuel ratio and steam/fuel ratio on gasification characteristics were investigated. Although, the increase of air inlet temperature was the only way to increase the producer gas calorific value and cold gas efficiency, it also increased the gasification temperature which was not favorable. Steam injection was found to reduce the gasification

temperature and increase the H_2/CO ratio, a finding rarely reported in the literature. The developed model in this study can be used to simulate gasification of other types of biomass materials and predict the effect of important variables in optimization of a biomass downdraft gasifier.

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