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چکیده فارسی

مدلسازی عددی فرایند گازی سازی زیست توده ها؛

ارائه روشی جایگزین برای فرایند احتراق

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مقاله حاضر به ارائه یک مدل عددی بر پایه تعادل ترموشیمیایی پرداخته و با بهره گیری از آن، عملکرد یک راکتور گازی سازی پایین سو را پیش بینی کرده است. داده های عددی حاصل، در مقایسه با نتایج تجربی، از دقت قابل قبولی برخوردارند. در جریان شبیه سازی فرایند گازی سازی به کمک مدل عددی تولید شده، زیست توده های متنوعی مورد ارزیابی قرار گرفتند که در میان آنها، پسماندهای جنگلی به عنوان انرژی زاترین زیست توده برگزیده شدند و مطالعات مربوط به سنجش عملکرد راکتور، بر روی آنها انجام گرفت. در جریان مطالعات، تاثیر شرایط عملیاتی شامل محتوای رطوبت، نسبت بخار به سوخت، نسبت هوا به سوخت و دمای هوای ورودی بر مشخصه های گازی سازی مورد سنجش قرار گرفت. مشخصه های گازی سازی مورد اشاره عبارت بودند از: دمای گازی سازی، ترکیب مولفه های گاز سنتزی و ارزش گرمایی گاز سنتزی. در این میان آشکار شد که تغییر دمای هوای ورودی، یگانه روش افزایش همزمان ارزش گرمایی گاز سنتزی و راندمان گازی سازی است. از سوی دیگر مشخص شد که نسبت بخار به سوخت، نقشی کلیدی در کنترل دمای گازی سازی و تنظیم نسبت هیدروژن به مونواکسید کربن بر عهده دارد. مدل عددی تولید شده را می توان به عنوان ابزاری برای طراحی شرایط اولیه و عملیاتی راکتورهای گازی سازی، هم چنین به منظور بهینه سازی عملکرد آنها به کار گرفت.

واژگان کلیدی: گازی سازی، تعادل ترموشیمیایی، مدلسازی عددی، انرژی های تجدید پذیر، زیست توده ها

(i.e. biomass and moisture). Evaluating the energy of the produced syngas and that of the feedstock in the same state (reference temperature), the cold gas efficiency can be 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 in cold gas efficiency, other parameters have a reverse effect.

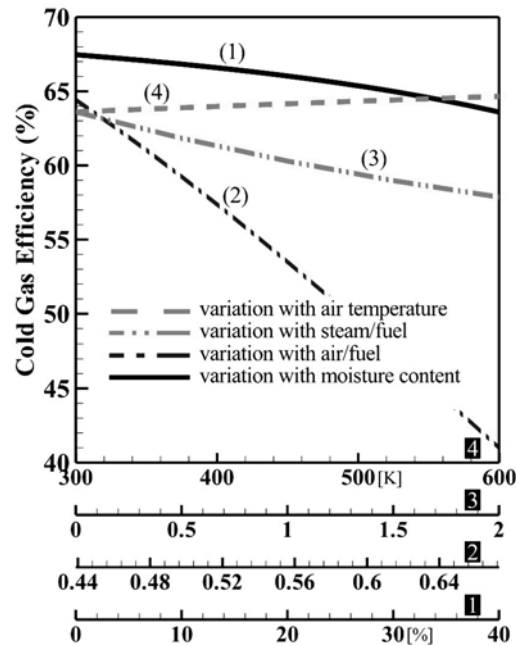


Fig 6. Influence of four effective parameters on cold gas efficiency

Conclusion

A thermodynamic equilibrium model was developed for a biomass gasifier in order to calculate the composition of the produced syngas, and investigate the gasification characteristics. The predicted results agreed well with those of the experiments available in the literature. The model 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 in air inlet temperature was the only way to increase the produced syngas 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 H₂/CO ratio. 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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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 produced syngas. For an increase in air temperature from 300K to 600K, the produced syngas composition was not changed considerably; however, the calorific value was increased by 0.6% and the gasification temperature by 130 K. The slight increase of calorific value (only 0.6%) does not justify the increase in the air inlet temperature because of the considerable rise in the gasification temperature (by 130 K), 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 approaches the usual combustion level with a tendency to produce CO_2 and N_2 (dominant products of combustion process). This will increase the temperature and considerably decreases the calorific value of the produced syngas.

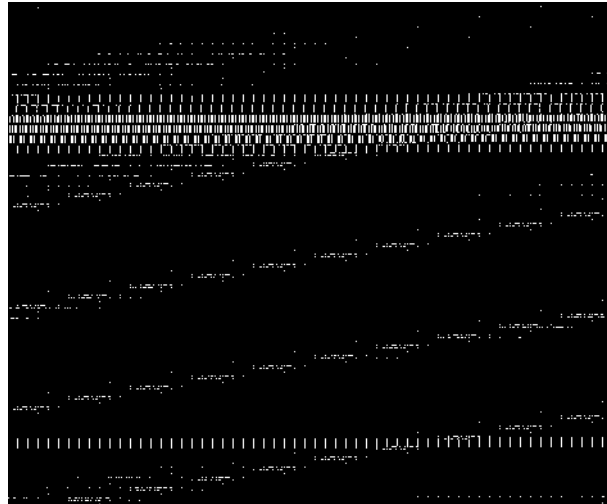


Fig 4. Effect of air/fuel ratio on gas composition

The effect of steam/fuel ratio on the calorific value of the produced syngas and the gasification temperature is shown in Fig.5. Steam in gasification is called "moderator" as it can be used as a means for controlling the gasification temperature (see Fig. 5). In addition, it can be used to adjust H_2/CO ratio and increase the volume of CH_4 in the produced syngas.

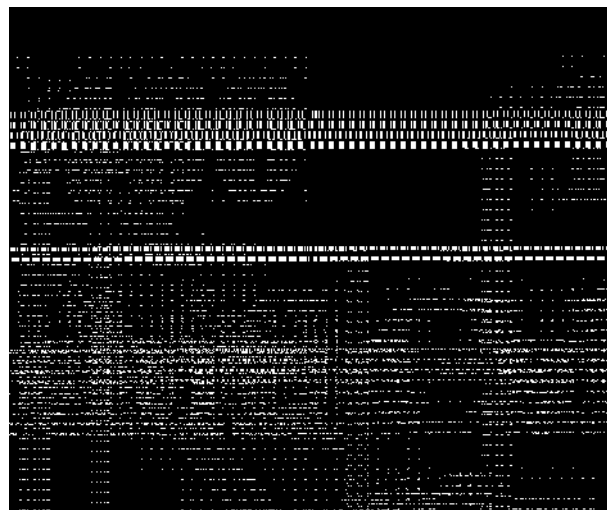


Fig 5. Effect of steam/fuel ratio on calorific value of the produced syngas and gasification temperature

Finally, we study the influence of four effective parameters on cold gas efficiency (also known as the first law of thermodynamic efficiency) defined as the ratio of the energy leaving the gasifier to the energy entering it

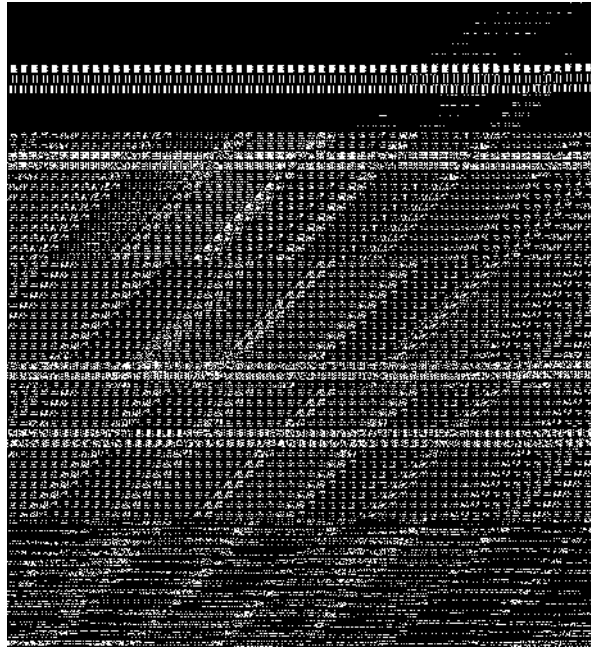


Fig 1. Comparison between calorific values obtained via gasification of 20 different biomass materials [18]



Fig 2. Effect of moisture content on gas composition

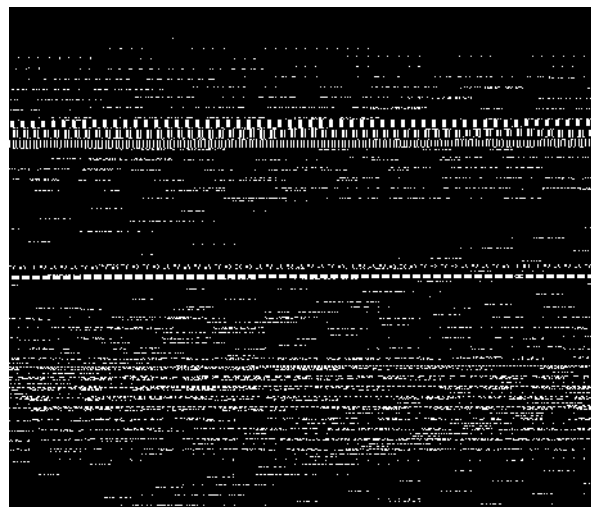


Fig 3. Effect of moisture content on gasification temperature and calorific value of the produced syngas

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

When the equilibrium constants are defined, a system of equations will be obtained, which needs 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 produced syngas 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.

Results and discussion

In this section, the results of the presented model for produced syngas 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 the methane are slightly less than those in 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. 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 - ^c $RMS = \sqrt{\frac{\sum_i^N (Exp_i - Num_i)^2}{N}}$

National Renewable Energy Laboratory of the United States has published chemical properties of 55 biomass materials [18]. In order to compare various biomass sources of energy, gasification of 20 different samples of them is simulated under the same conditions (biomass with zero moisture content and stoichiometric coefficient equal to 0.46) to evaluate their produced syngas calorific values. These samples were selected across five major groups 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 as well as the storing and transportation conditions. Therefore, analyzing the effect of moisture content on produced syngas composition and gasification characteristics is of great importance. The effect of moisture content on the produced syngas 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, and yet 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 the figure that increasing the moisture content reduces the calorific value of the produced syngas. 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 in CO is greater than the increase in H₂, the resultant calorific value of the produced syngas is decreased. Figure 3 also shows that increasing the moisture content reduces the gasification temperature. This is because a greater moisture content means that more energy is required for vaporization. The above results are in good agreement with the numerical results of Zainal et al. [9] and Jarunthammachote et al. [16].

where x_i is mole fraction of the species i in the ideal gas mixture, ν is the stoichiometric number, P_0 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:

$$K_1 = \frac{(n_{CO_2})^{(n_{H_2})}}{(n_{CO})^{(n_{H_2O})}} \quad (9)$$

$$K_2 = \frac{(n_{CH_4})}{(n_{H_2})^2} \frac{1}{P} \quad (10)$$

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

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

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

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

where h_f^D 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:

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

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

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

The amounts of ΔG^D and h_f^D can be found in chemical engineering handbooks [17]. Jarungthammachote 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 which is 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:

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

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

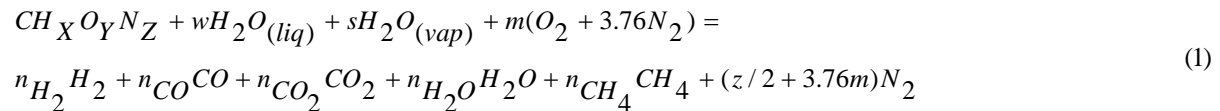
$$\Delta h_T^D = \int_{298}^T \bar{C}_p(T) dT \quad (16)$$

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]:

analysis on the calorific value is studied for 20 different common biomass materials and the most energetic one is selected as a sample for the 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 and its calorific value, gasification temperature, and the cold gas efficiency.

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 a chemical equilibrium. In addition, all carbon in the biomass is assumed to be gasified and, therefore, the formation of char is negligible. 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 °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]:

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

M_{bm} and M_{H_2O} are the masses of the biomass and the 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. Moreover, the enthalpy of formation for biomass can be obtained as follows [14]:

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

where $h_{f,i}^D$ 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 produced syngas, 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:

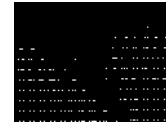


Higman and van der Burgt [15] showed that Eqs.(4) and (5) can be combined to give the water–gas shift reaction as:



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:

$$K = \prod_i (x_i)^{v_i} \left(\frac{P_0}{n_{total}} \right)^{\sum_i v_i} \quad (8)$$



On a Numerical Model for Gasification of Biomass Materials: An Alternative Method to Combustion

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In this paper, a thermochemical equilibrium model is used to predict the performance of a downdraft biomass 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 syngas calorific value and cold gas efficiency. The steam/fuel ratio, on the other hand, plays a key role in controlling the gasification temperature and H₂/CO ratio.

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

Introduction

Biomass as a new source of energy has drawn world-wide attention during the last decade. Positive rate of consumption of fossil fuels, and the negative rate of their natural reservoirs as well as restricting environmental concerns urge the need to find alternative sources of fuel such as biomass. Byproducts of activities like agriculture or food processing are categorized as biomass materials. These materials used to be disposed of in open lands create 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 a synthesis gas (syngas), mainly comprising of H₂, CO, and CH₄. One of the attractive features of this technology includes the ability to produce a clean syngas product that can be used either for generating electricity or producing chemicals.

It must be emphasized 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 so as 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 the calorific value typically at 6-12 MJ/m³ (natural gas is 34 MJ/m³) and 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, and 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 in reality, thermodynamic equilibrium never takes place in a gasification process [5], several works were performed to demonstrate the applicability of the equilibrium model to this process. These models especially work well in high temperatures that occur in entrained flow gasifiers (above 1500 K) [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 syngas composition as a function of the fuel/ air ratio by means of an equilibrium model. A description of a 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 with a comparison between the calculated results and the two separate experiments available in the literature [2,4]. The effect of ultimate

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