



Effects of various operational parameters on biomass gasification process; a modified equilibrium model



Hojat Ghassemi, Rasoul Shahsavan-Markadeh *

School of Mechanical Engineering, Iran University of Science and Technology, Narmak, Tehran 16846-13114, Iran

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ABSTRACT

In this paper by means of a modified equilibrium model based on Gibbs free energy minimization, performance of biomass gasification process is studied. Effects of parameters such as equivalence ratio, gasification temperature, fuel type and its moisture content, and gasifying agent, are investigated. Model results show that temperature has significant influence on cold gas efficiency more remarkably at lower temperature and has negligible effect on syngas heating value. Enriching the air with O₂ increases gas higher heating value (HHV) and for larger amount of oxygen it shows a maximum as equivalence ratio increases. Cold gas efficiency for higher oxygen amount is larger and its maximum obtained at lower equivalence ratio. By increasing the H/C molar ratio of biomass, cold gas efficiency increases but biomass O/C ratio shows adverse effect. Moisture content of biomass has negative effects on cold gas efficiency and HHV. For higher equivalence ratio this negative effect decreases.

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1. Introduction

Biomass as a renewable, widely available and CO₂-neutral energy resource, is the third largest primary energy resources after coal and oil. It provides 14% of the world's annual energy consumption [1]. Gasification which converts biomass to syngas with various applications, is one of the promising technologies which has many advantages over direct combustion [2].

The gasification is a chemical process that converts the solid or liquid fuels into gaseous fuel using gasifying agents such as air and oxygen. Based on how and where gasifying agent and fuels meet each other, there are three major types of gasifiers; fixed bed, fluidized bed, and entrained flow. Fluidized bed gasifiers, that have good heat and mass transfer between gas and solid phase and tolerate variations in fuel quality and particle size [3], are one of the suitable technologies for biomass conversion. Many parameters can affect biomass gasification performance, such as reactor pressure and temperature, fuel quality, type of gasifying agent, particle size. Some researchers studied the effects of various parameters through experiments [4–6]. Many models, also are developed for biomass gasification in fluidized bed gasifiers which Gomez-Barea and Leckner presented a comprehensive review of them [7]. Models can be categorized into three types; equilibrium, finite rate, and neural network models [8]. Equilibrium models due to their simplicity and few input requirements are suitable for preliminary studies and are widely used by researchers [9–14]. Due to

existence of non-equilibrium phenomena in the gasifier, equilibrium models results differ from experimental data. Hence, some of modelers applied modifications on their models to obtain better agreement between predicted and actual results. Li et al. assumed complete conversion for all elements other than carbon and hydrogen and imposed an availability function on these two elements to modify element abundance vector [15]. Jarungthammachote and Dutta considered heat loss to be 1% of the higher heating value of biomass and modified the model by considering carbon conversion of 60% [16]. Barman et al. in their equilibrium model assumed 4.5% of product to be tar and consider its formula as CH_{1.003}O_{0.33} [17]. These kinds of modification lead to better agreement between models and experiments.

By means of equilibrium models various parameters effects are investigated. Antonopoulos et al. developed a non-stoichiometric equilibrium model and studied effects of moisture content and temperature on syngas quality [18]. Altafini et al. studied effects of various parameters on wood gasification by means of an equilibrium model [19]. Aspen Plus simulation based on Gibbs free energy minimization, was used to study effect of air preheating on performance of a circulating fluidized bed biomass gasifier [20]. Schuster et al. perform an extensive parametric study and surveyed influences of parameters such as temperature, fuel composition and amount of fluidizing agent. [21].

In this study a modified equilibrium model based on Gibbs free energy minimization approach is presented. Modifications for carbon conversion and tar formation are applied. Effects of gasification parameters such as equivalence ratio, process temperature, fuel type and its moisture content, and gasifying agent are studied.

* Corresponding author. Tel.: +98 913 2324628.

E-mail address: rsahsavan@mecheng.iust.ac.ir (R. Shahsavan-Markadeh).

Nomenclature

C_p	specific heat at constant pressure
G	total Gibbs free energy
h_f^0	enthalpy of formation
\bar{H}	total enthalpy
HHV	higher heating value
LHV	lower heating value
\dot{m}	mass flow rate
n	number of moles
N	number of species
NG	number of gaseous species

P	pressure
Q	heat exchange
R	gas constant
T	temperature

Greek letters

δ_c	carbon conversion efficiency
φ	equivalence ratio
η_{cg}	cold gas efficiency
μ	chemical potential

Performance of gasification process is determined by syngas higher heating value and gasification cold gas efficiency. By studying the effects of gasification parameters on optimum condition this idea that if gasifying agent consumption varies for different operating condition, is investigated.

2. Model description

Thermodynamic equilibrium calculations based on Gibbs free energy minimization is chosen to model biomass gasification process. In thermochemical equilibrium state total Gibbs free energy of system is minimum [22]. The total Gibbs free energy of system is defined as follows

$$G = \sum_{i=1}^N n_i \mu_i \quad (1)$$

where μ_i and n_i are chemical potential and number of moles of i th species, respectively. Chemical potential is defined as [23]:

$$\mu_i = \left(\frac{\partial G}{\partial n_i} \right)_{T,P,n_{j \neq i}} \quad (2)$$

For gas phase ($i = 1, 2, \dots, NG$) and condensed phase ($i = NG + 1, \dots, N$) chemical potential can be calculated as follows [24]:

$$\mu_i = \begin{cases} \mu_i^0 + RT \ln \frac{n_i}{n_{tot}} + RT \ln \frac{P}{P^0} & i = 1, 2, \dots, NG \\ \mu_i^0 & i = NG + 1, \dots, N \end{cases} \quad (3)$$

where P , T , R , and n_{tot} are pressure, temperature, gas constant, and total number of moles, respectively and “o” superscript means standard conditions. μ_i^0 is the chemical potential at standard conditions and equals to Gibbs energy of formation at given temperature which can be calculated as follows:

$$\Delta G^0 = \Delta H^0 - T \Delta S^0 \quad (4)$$

where ΔH^0 and ΔS^0 are enthalpy and entropy of formation at the given temperature. For minimizing Gibbs free energy under following constraint,

$$\sum_{i=1}^{NS} a_{ji} n_i - b_j^0 = 0 \quad (5)$$

Lagrange multiplier method is used and final equations obtained as follows:

$$\left(\mu_i + \sum_{j=1}^{NE} \lambda_j a_{ji} \right) = 0 \quad (6)$$

$$\sum_{i=1}^{NS} a_{ji} n_i - b_j^0 = 0 \quad (7)$$

$$\sum_{i=1}^{NS} n_i = n_{tot} \quad (8)$$

where a_{ji} and b_j^0 are number of atoms of element j in species i and number of moles of element j in reaction, respectively. NE, NS, and λ_j are respectively, number of elements, number of species, and Lagrange multiplier.

According to the first law of thermodynamics, enthalpy equation is obtained as:

$$H_P = H_R + Q_{in} - Q_{out} \quad (9)$$

Q_{in} and Q_{out} are exchanges of heat between reactor and surrounding which is neglected in this study. H_P and H_R are enthalpy of products and reactants, respectively. Assuming the ideal gas behavior, enthalpies are temperature dependent and can be calculated by means of each species enthalpy at given temperature.

$$H_{R,P} = \sum_{R,P} n_i \bar{h}_{f,298}^0 + \sum_{R,P} n_i \int_{298}^{T_i} C_{pi} dT \quad (10)$$

where C_{pi} and $\bar{h}_{f,298}^0$ are specific heat and enthalpy of formation of i th species. In order to calculate the thermodynamic properties of species, such as Gibbs energy and enthalpy, at a specific temperature following equations are used [25].

$$\frac{H_T^0}{RT} = -a_1 T^{-2} + a_2 \frac{\ln T}{T} + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{b_1}{T} \quad (11)$$

$$\frac{S_T^0}{R} = -a_1 \frac{T^{-2}}{2} + \frac{a_2}{T} + a_3 \ln T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + b_2 \quad (12)$$

where coefficients of this equation are available for several species [25].

Enthalpy of formation of biomass is calculated by means of its heating value [26]:

$$\bar{h}_{f,biomass}^0 = LHV_{biomass} + \sum_k n_k \bar{h}_{f,k}^0 \quad (13)$$

where $\bar{h}_{f,k}^0$ is the enthalpy of formation of product k under complete combustion of biomass. Heating value of biomass in terms of MJ/kg can be determined by knowing its elemental analysis [27].

$$HHV = 0.3491C + 1.1783H + 0.1005S - 0.1034O - 0.0151N - 0.0211A \quad (14)$$

where C, H, S, O, N, and A are mass percentage of carbon, hydrogen, sulfur, oxygen, nitrogen, and ash in dry biomass, respectively. For calculation of LHV of biomass following correlation is used [16]:

$$LHV = HHV - 9m_H(h_{fg}) \quad (15)$$

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