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On the Thermo-Chemical Equilibrium Modelling of a Biomass Gasifying Process

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ABSTRACT

This article discusses a mathematical model for the thermochemical processes in a downdraft biomass gasifier. The model combines the chemical equilibrium and the thermodynamic equilibrium of the global reaction, predicting the final composition of the producer gas as well as its reaction temperature. Once the composition of the producer gas is obtained, a range of parameters can be derived, such as the cold gas efficiency of the gasifier, the amount of dissociated water in the process and the heating value and engine fuel quality of the gas. The model has been validated experimentally. This work includes a parametric study of the influence of the gasifying relative fuel/air ratio and the moisture content of the biomass on the characteristics of the process and the producer gas composition. The model helps to predict the behaviour of different biomass types and is a useful tool for optimizing the design and operation of downdraft biomass gasifiers.

KEYWORDS: mathematical model, thermodynamic equilibrium.

1. Introduction

Gasification is an attractive technology for the thermo chemical valorization of biomass. There is an increasing interest in the use of biomass for heat and power production considering the growing concern for future energy supply.

The aim of this work was to develop an equilibrium gasification model using Matlab code and to validate the model using data of gasifiers used for wood biomass in the literature.

The equilibrium models can predict the exit gas composition, given the solid composition and the equilibrium temperature based on the assumption that the gasifier reactions are in thermodynamic equilibrium.

Melgar et al. (2007) presented a biomass gasification model by means of chemical equilibrium, minimizing the Gibbs free energy in which the influence of the gasifying agents/fuel ratio and humidity on the equilibrium temperature (adiabatic case) was analyzed.

Jayah et al.(2003) have built a two zone model. The two zones correspond to flaming pyrolysis and the gasification. In the flaming pyrolysis zone, the producer gas composition was estimated by a chemical equilibrium. These parameters form the input of the second zone.

In all these works, as for all equilibrium models, a set of non-linear equations describing the conservation of chemical species (C, O, H, N, S) and the additional equations for thermal equilibrium of the independent reactions (which corresponds to the minimization of the free energy of reaction) allows a prediction of the output under a given composition of the reactants and operating conditions (pressure and temperature).

In a reversible chemical reaction at a given time under specified conditions of temperature and pressure a state of dynamic equilibrium is determined, characterized by an unchanging composition over time.

A steady state is established when the speeds at which the performance of the two opposing reactions are equal and simultaneous.

For reversible chemical reaction of the form:

$$\sum_{i=1} \nu_i A_i \leftrightarrow \sum_{i=1} \nu' A'_i \,, \qquad (1)$$

The direct reaction rate is:

$$v_1 = k_1 \prod_{i=1}^{n} C_{A_i}^{\nu_i} \,, \qquad (2)$$

The reverse reaction rate is:

$$v_2 = k_2 \prod_{i=1}^{n} C_{A_i}^{\nu_i} , \quad (3)$$

In these conditions, in a steady state, we can write

$$k_1 \prod_{i=1}^{n} C_{A_i,ech}^{\nu_i} = k_2 \prod_{i=1}^{n} C_{A_i',ech}^{\nu_i'} , \quad (4)$$

thus

$$K_c = \frac{k_1}{k_2} = \frac{\prod_{i=1}^{n} C_{A_i',ech}^{\nu_i'}}{\prod_{i=1}^{n} C_{A_i,ech}^{\nu_i}} \quad (5)$$

where: k1 and k2 is the rate constant for the reaction of one mole of reactant (s) and the reaction product, Kc, the equilibrium constant of reaction being expressed in units of molar concentrations.

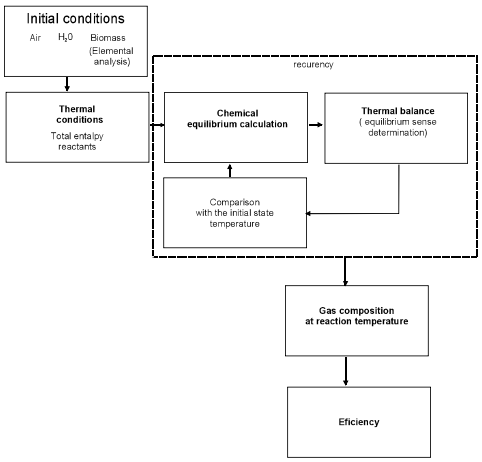

Fig 1. *Schematic procedure approaching*

Equation (4) defines the mass action law (Guldenbeg and Waage), which establishes the interdependence between the equilibrium concentrations of substances participating in the reaction temperature and the time pressure (for gaseous systems containing chemicals).

The equilibrium constant depends on temperature, pressure and concentration of the reactants and the products at the equilibrium response.

According to Le Chatelier's principle, the principle of chemical equilibrium movement, if one of the factors that influence changes the chemical balance, the system moves to a new position of equilibrium in the sense that opposes change products.

This means that the increasing concentration of a reactant, the addition of the chemical system, moving balance, for the purposes of consumption, so a direct response.

The decrease in concentration of reaction product by removing it from the system displaces the equilibrium in the sense of training, so the direct reaction.

This paper presents a preliminary result in our effort to build a Matlab code well adapted to model of the gasification process (equilibrium) for different type of biomass.

In this paper, we study the influence of the concentration on chemistry by doing the following reaction of the form:

$$CH_xO_yN_z + m_wH_2O + x_g(O_2 + 3.76N_2) \rightarrow x_1CO + x_2H_2 + x_3CO_2 + x_4H_2O + x_5CH_4 + \left(\frac{z}{2} + x_g 3.76\right)N_2 \quad (6)$$

From the global reaction there results a system of six equations with six variables x_1, x_2, x_3, x_4, x_5, which represent five species of products and oxygen content for reactions.

Six equations are required based on the atomic balance (Carbon balance, Hydrogen and Oxygen balance):

$$x_1 + x_3 + x_5 = 1 , \quad (7)$$

and

$$x + 2m_w = 2x_2 + 2x_4 + 4x_5 , \quad (8)$$

and respectively

$$y + m_w + 2x_g = x_1 + 2x_3 + x_4 , \quad (9)$$

The equilibrium constants as related to the molar composition can be written as follows:

$$K_1 = \frac{P_{CO_2} \cdot P_{H_2}}{P_{CO} \cdot P_{H_2O}} = \frac{n_{CO_2} \cdot n_{H_2}}{n_{CO} \cdot n_{H_2O}} = \frac{x_3 x_2}{x_1 x_4} , \quad (10)$$

and

$$K_2 = \frac{P_{CH_4}}{\left(P_{H_2}\right)^2} = \frac{n_{CH_4} \cdot n_{tot}}{n_{H_2}^2} = \frac{x_5}{x_2^2} n_{tot} , \quad (11)$$

2. Description of the Modeling of the Gasification Process

The following hypotheses were considered to draw the model:

- The process is in adiabatic conditions.
- This process was supposed to occur instantaneously at equilibrium with volatile products mainly made of H_2, CO, CO_2, CH_4 and H_2O.
- Tars are assumed to be negligible in the syngas and are not taken into account in this study.

3. Matlab Model and Specific Results

The algebraic method is one of the most used procedures to resolve systems of nonlinear equation in Matlab.

In this way, the algorithm has some elementary parts:

1. The model requests the preliminary elemental composition and the work temperature
2. the software computes the Gibbs potential variations in order to succeed in reaching the process temperature evolution
3. in the third stage, the program succeeds in building the linear equation system and obtains the find syngas composition in dry syngas basis
4. evaluate the process temperature and subtracts the evolution sense of the chemical reaction
5. using the energy balance could be found the next step temperature variation

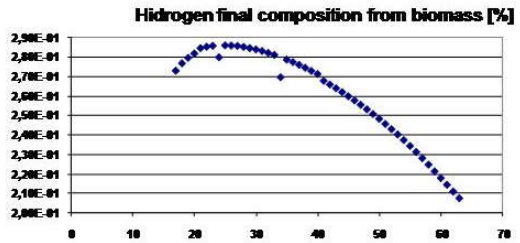

Fig. 2. *Hydrogen composition from biomass versus carbon composition [%]*

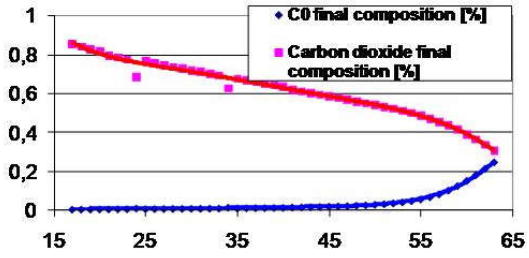

Fig. 3. *Carbon dioxide and Carbon mono-oxide composition versus carbon composition from biomass [%]*

4. Model Validation and Discussions

The model presented in this article has been compared to the experimental and predicted producer gas presented by Jayah (2002).

The proximate and ultimate analyses of rubber wood used in these experiments are given in Table 1. The moisture content of rubber wood is 18.2% defined on a dry mass basis.

Table 1. *Proximate analysis and ultimate analysis of rubber wood.*

Proximate	Wt % dry basis	Ultimate	Wt % dry basis
Volatile matter	80.1	C	50.6
Fixed carbon	19.2	H	6.5
Ash	0.7	O	42
		N	0.2
		Ash	0.7

Table 2. *Preliminary comparison for our model*

	Jayah (2002)		Melgar (2007)		This work
	Model	Work	Model	Work	Model Matlab
H_2	16.6	17.6	16.4	15.5	8,04
CO	19.2	19.3	18.3	19.1	22,58
CO_2	11	11.1	11.2	11.4	15,48
CH_4	0.2	0.4	1.1	1.1	16,76
N_2	53	51.6	53.2	52.9	37,14

5. Conclusions

In this study, a thermochemical equilibrium model for downdraft has been proposed. The model using Matlab code is easy to build and predicts with accuracy the composition of the producer gas.

The reaction temperature is the parameter that controls the whole gasification process. It influences directly the final producer gas.

An optimal temperature has to be found between a too high temperature process corresponding to a gas with a low calorific value and a low temperature process where the gas contains tar because the exit gas is not at equilibrium.

Concentrations given by the producer gas model can, in this case, be used as input data to the combustion model in the Fluent code.

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Studiu asupra modelării echilibrului termo - chimic pentru un proces de gazeificare

Rezumat

Acest articol prezintă un model matematic pentru procesele termochimice într-un gazeificator de biomasă. Modelul combină echilibrul chimic şi echilibrul termodinamic de reacție, estimează compoziția finală a produselor de gaze, precum şi temperatura de reacție. Odată ce conținutul de gaze de produse este obținut, o serie de parametri pot fi calculați, cum ar fi eficiența gaz rece de gazeificare, cantitatea de apă disociată în procesul de încălzire şi de valoarea şi calitatea de carburant al motorului de gaz. Modelul a fost validat prin comparație. Acest lucru include un studiu parametric de influenta de combustibil relativ gazeificare / raportului aer şi conținutul de umiditate al biomasei asupra caracteristicilor procesului şi compoziția gazului de producători.