Modeling Downdraft Gasification with use of A Predictive Pyrolysis Model

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Introduction

This paper presents a developed zero-dimensional mathematical model for downdraft gasification of biomass in fixed or slowly moving beds. Comparing with different gasification models found in literature, the proposed model involves main gasification sub-processes (drying, pyrolysis, gasification) and their products. The developed model has been validated with published experimental data from different authors, showing good agreement between reported data and results obtained from the model.

Methodology

A real gasification system differs from an ideal reactor at chemical equilibrium. For this reason, the pure thermodynamic equilibrium model, described elsewhere [1-4], has been modified to increase the results' accuracy. The gasification model consists of a series of sub-processes, each containing one process (biomass drying, pyrolysis, gasification, air preheating, and steam generation), see Figure 1.
The following assumptions were made:
1.Adding a drying unit, that predicts the removal of moisture from raw biomass. The percentage of removed moisture can alternatively be set by the user.
2.Adding a pyrolysis unit that, using empirical correlations, predicts the formation of pyrolysis products (charcoal and volatiles, including tar)
3.Adding tar and charcoal leaving the gasifier as a percentage of tar and charcoal produced in the pyrolysis unit [10]
4.Particles leaving the gasifier are set by the user as mg/Nm3 in the produced gas. These particles are considered to consist only of carbon.
5.Biomass--bound nitrogen, during gasification process is converted into a diatomic nitrogen gas (N_2).
6.Gas products consists of CO_2, CO, H_2, CH_4, N_2, and H_2O
7.Setting the amount of produced CH_4 = 2 vol% as an initial guess, needed for iteration process
8.No heat losses are considered from the gasifier, i.e. adiabatic condition
9.The air for the gasification process is considered as dry air, containing only 21% O_2 and 78% N_2 (volume fractions)
10.Biomass is assumed to enter the gasification at 25 °C and 1 atm.
The objectives of this model are:
1.To define and predict characteristics of the downdraft biomass gasification process,
2.To predict the yields of gas, charcoal, and tar produced during gasification,
3.To predict the composition of the gas covering conditions typically found in gasification, including pyrolysis (350-950ºC),

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4.To evaluate the influence of main input variables, such as moisture content and air/fuel ratio, temperature of the process, gasifying medium, etc.
Regarding this, an empirical predictive model is developed to describe the general trends of product distribution as a function of temperature, which is based on balance of elements, energy balance and empirical relationships.

The overall mass balances

The overall mass balance for the biomass gasification process is outline in Figure 1.

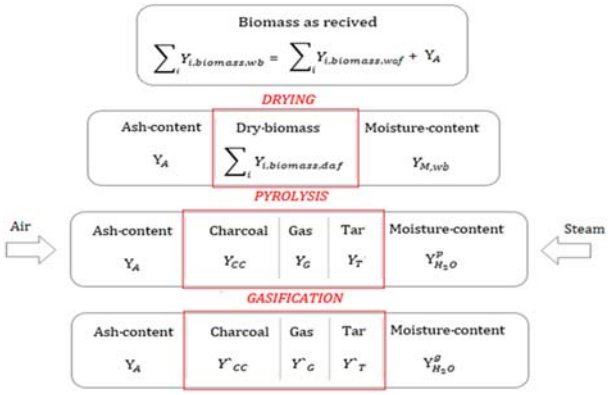

Fig. 1 Overall mass balance for the biomass gasification process

Gasification sub-processes can be described with the equations:
Drying:

$$\sum_i Y_{i,biomass,waf} + Y_A \xrightarrow[drying]{} \sum_i Y_{i,biomass,daf} + Y_{M,wb} + Y_A \quad (1)$$

where $\sum_i Y_{i,biomass,waf}$ is the mass fraction of the ith element (carbon, hydrogen, oxygen, nitrogen) in wet biomass on an ash free basis, Y_A is the ash content in biomass on dry basis, $\sum_i Y_{i,biomass,daf}$ is the mass fraction of the ith element (carbon, hydrogen, oxygen, nitrogen) in dry biomass on an ash free basis, $Y_{M,wb}$ is the moisture content of biomass in dry ash free basis.
Pyrolysis [5]:

$$\sum_i Y_{i,biomass,daf} + Y_{M,wb} + Y_A \xrightarrow[pyrolysis]{} \sum_j Y_{j,products,daf}^p + Y_{H_2O}^p + Y_A \quad (2)$$

where $\sum_j Y_{j,products,daf}^p$ is the mass fraction of jth pyrolysis product (charcoal, tar and gas) on a dry ash free basis, $Y_{H_2O}^p$ the moisture content in gas obtained in the process of pyrolysis.
The pyrolysis products and gas composition can be represented by equations 3 and4 [5]:

$$\sum_j Y_{Y\,j,products,daf}^p = Y_{CC} + Y_T + Y_G \quad (3)$$

$$Y_G = Y_{CO2} + Y_{CO} + Y_{CH4} + Y_{H2} \quad (4)$$

were Y_{CC}, Y_T, Y_G are the mass fraction of pyrolysis products (charcoal, tar and gas) on dry ash free basis, $Y_{CO2}, Y_{CO}, Y_{CH4}, Y_{H2}$ are the mass fraction of different gases (CO_2, CO, CH_4 and H_2) on dry basis. The assumption of this model is that, due to lower pyrolysis temperature, bio-mass-N was mainly converted into tar-N part and the charcoal-N.
For prediction of pyrolysis products, empirical relationships between the product yield and pyrolysis temperature are used (equations 5-11). The determination of empirical relationships between the product yield and pyrolysis temperature are explained in detail by Trninic et al. [5].

Temperature dependent charcoal, tar and gas yields are given by [5].

$$Ycc = 7.97T^2 \cdot 10^{-5} - 0.125 \cdot T + 68.87 \tag{5}$$

$$Y_T = -1.38T^2 \cdot 10^{-4} + 0.12 \cdot T + 12.64 \tag{6}$$

$$Y_G = 1.12T^2 \cdot 10^{-4} - 0.058 \cdot T + 30.77 \tag{7}$$

Dependence of gas yield on pyrolysis temperature is described by [5]:

$$Y_{CO} = -2.65T^2 \cdot 10^{-4} + 0.27 \cdot T - 32.71 \tag{8}$$

$$Y_{CO2} = -2.85T^2 \cdot 10^{-5} - 0.029 \cdot T + 70.89 \tag{9}$$

$$Y_{CH4} = 6.69T^2 \cdot 10^{-5} - 0.037 \cdot T + 4.28 \tag{10}$$

$$Y_{H2} = 7T^2 \cdot 10^{-5} - 0.0371T + 5.1117 \tag{11}$$

In addition to these correlations, the energy, mass, and molar balances for each element are set and used to calculate pyrolysis products. The elements considered are C, H, O, and N. S is neglected due to its small amount. Other elements are lumped as ash.

Gasification:

$$\sum_j Y^p_{j,products,daf} + \mathrm{Y}^p_{H_2O} + Y_A + \mathrm{Y}_{AIR} + \mathrm{Y}_{STEAM} \xrightarrow[gasification]{} \sum_j Y^g_{j,products,daf} + \mathrm{Y}^g_{H_2O} + Y_A \tag{12}$$

where Y_{AIR} is the mass fraction of air, Y_{STEAM} is the mass fraction of steam, $\sum_j Y^g_{j,products,daf}$ is the mass fraction of jth gasification product (charcoal, tar and gas) on a dry ash free basis, $\mathrm{Y}^g_{H_2O}$ is the moisture content in gas obtained in the process of gasification.

The gasification products and gas composition can be represented by equations 13 and 14:

$$\sum_j Y^g_{Y_{j,products,daf}} = Y`_{CC} + Y`_T + Y`_G \tag{13}$$

$$Y`_G = Y`_{CO2} + Y`_{CO} + Y`_{CH4} + Y`_{H2} + Y`_{N2} \tag{14}$$

where $Y`_{CC}, Y`_T, Y`_G$ are the mass fraction of charcoal, tar and gas on a dry ash free basis, while $Y`_{CO2}, Y`_{CO}, Y`_{CH4}, Y`_{H2}, Y`_{N2}$ are the mass fraction of the different gases (CO_2, CO, CH_4, H_2 and N_2) on dry basis produced after the gasification process.

The three most common gas–solid reactions that occur in the gasification zone considered in modeling are: the water–gas or steam reaction, the Boudouard reaction and the methanation reaction. The equilibrium constants for all considered reactions are defined by corresponding mole fractions and theirs temperature correlations are provided according to the literature data.

In addition to these correlations, the energy, mass, and molar balances for each element (C, H, O, and N) are set and used to calculate the gasification products. An initial gasification temperature is assumed in the iterative solution procedure.

Validation of the model

The "Engineering Equation Solver (EES)" has been found to be very suitable for modelling this kind of system, because it contains all of the necessary thermodynamic functions and it is possible for the model builder to make a user interface, which can make the model user-friendly [10].

Model (operating) parameters (biomass characteristics (proximate analyses and the elemental compositions), drying temperature, percentage of removed moisture, pyrolysis temperature, air inlet temperature, steam inlet temperature, gasification temperature and percentage of charcoal, tar and particles leaving the gasifier) can be directly introduced by the user.

The results obtained with the model are validated with those obtained experimentally by different authors for different kinds of biomass [6-9]. Predicted results from the present modified equilibrium model are presented in Table 1.

The model predicted most of the measured yields within ±15% accuracy, and the prediction was often within the uncertainty of the measurements. In general, the present model gives smaller volume fractions of CH_4 and slightly higher volume fractions of H_2 than the experimental results given by da Silva. Amount of CH_4 was set by the user (initial guess values 2 vol%). Knowing that with increasing CH_4 the amount of H_2 decreases, the proportions of results obtained from the model are reasonable.

Conclusion

The gasification model is made up of a series of submodules, each containing one process. An overall scheme is adopted by considering the different steps in which the gasification process can be approximately subdivided: heating and drying, pyrolysis or devolatilization, partial oxidation, and reduction (or charcoal gasification The fundamental equations in the model are based on two conservation (mass and energy) laws. Determination of the gas composition from the gasification chamber is based on equations for element balances, the water gas shift reaction and the methanisation reaction.

This model has been validated with published experimental data. For downdraft gasifiers, the predicted values for air gasification are in very good agreement with the experimental ones for all cases.

The developed model will be able to predict phenomena in a wide range of experimental conditions and for different types of biomass material with a defined ultimate composition and moisture content. The model can be used to predict the final producer gas composition and its heating value. Also, the model is accurate enough to predict the behaviour of downdraft fixed bed gasifiers for air and steam gasification.

The proposed model is a useful tool for preliminary calculations, design, and operation of biomass gasifiers. Also, this model can be used as input to a combustion model or as an input model for a whole biomass cogeneration plant.

Table 1 Comparison of gas composition given by the downdraft gasification model and results from literature review

	M[1]	da Silva [7]	δx^2 (%)	M	Arun et al [8]	δx (%)	M	Perez et al [9]	δx (%)	M	Jayah et al. [6]	δx (%)
Tg, °C	930	930		750	750		813	813		800	800	
ER	0.2	0.2		0.30	0.30		0.33	-		0.30	-	
biomass	corn cob			corn cob			pine bark			rubber wood		
CO, % vol	21.7	19	14.6	17.5	15.6	12.1	22.0	21.55	2.2	21.5	19.6	9.9
CO_2, % vol	10.7	10.3	4.2	14.9	14.3	3.8	10.2	11.1	7.6	8.6	10.8	19.9
H_2, % vol	16.1	15.9	1.3	17.7	15.6	13.3	13.7	16.7	17.7	18.5	16.4	13.0
CH_4, % vol	1.8	3	37.0	1.9	1.9	4.6	1.9	2.4	18.9	1.8	1.4	30
N_2, % vol	49.4	49.5	0.2	47.8	52.4	8.7	51.8	47.8	8.5	49.4	51.9	4.7

Note: ER can be set in the model; Air/Biomass is calculated by the model; 1 - M – Model values: 2 – δx – relative error

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