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DEVELOPMENT OF A NEW STOICHIOMETRIC EQUILIBRIUM-BASED MODEL FOR WOOD CHIPS AND MIXED PAPER WASTES GASIFICATION BY ASPEN PLUS

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ABSTRACT

Wood and paper residues are usually processed as wastes, but they can also be used to produce electrical and thermal energy through processes of thermochemical conversion of gasification. This study proposes a new steady state simulation model for down draft waste biomass gasification developed using the commercial software Aspen Plus for optimization of the gasifier performance. The model was validated by comparison with experimental data obtained from six different operation conditions. This model is used for analysis of gasification performance of wood chips and mixed paper wastes. The operating parameters of temperature and moisture content (MC) have been varied over wide range and their effect on the high heating value (HHV) of syngas and cold gas efficiency (CGE) were investigated. The results show that increasing the temperature improves the gasifier performance and it increases the production of CO and H_2 *which leads to higher LHV and CGE. However, an increase in moisture content reduces gasifier performance and results in low CGE.*

Keywords: waste biomass gasification, simulation model, Lower heating value, Cold gas efficiency

NOMENCLATURE

AFR	Air to fuel mass flow rate ratio, [kg_{air}/kg_{fuel}]
DCOALIGT	Density model for non-conventional components in ASPEN
CGE	Cold gas efficiency [%]
ER	Equivalence Ratio [%]
FC	Fixed carbon
Gp	Syngas yield, [m^3/kg fuel]
HCOALGEN	Enthalpy model for non-conventional components in ASPEN
HHV	Higher Heating Value, [J/m^3]
LHV	Lower Heating Value, [J/m^3]
MC	Moisture content [%]
MCINCPSD	Stream for non-conventional components in ASPEN, containing three substreams of MIXED, CIPSD and NCPSD class
R	Reaction
RE	Reactor
Sep	Separator
V	Volume, [Nm^3]
VM	Volatile matter
y	Mole fraction

1. INTRODUCTION

Increasing knowledge about the depletion of conventional energy sources and concern about environmental protection have encouraged the higher use of renewable energy alternatives [1]. Biomass as a renewable energy source, has obtained more interest because it is the only suitable and primary energy resource that can provide transportation fuels [2-4]. Biomass gasification is an attractive option that is getting huge attention for conversion of different feedstocks to energy. In gasification, waste like paper, cardboard, or wood is mixed with steam and oxygen at high temperature and is converted to syngas including mainly carbon monoxide and hydrogen. This gas is valuable in the chemical industry which can be used to produce solvents, plastics and fuels. Syngas can also be consumed directly as an energy source to generate power and hot water or steam.

Simulation of biomass gasification has been used to analyze the effect of various operating conditions on gasifier performance. The simulation can be performed using kinetic rate models or thermodynamic equilibrium methods. Thermodynamic equilibrium approaches are relatively simple and independent on gasifier design, which makes them more popular [5]. The thermodynamic equilibrium approaches are based on estimating the outlet compositions using different methods of stoichiometric and non-stoichiometric approaches. When implementing the stoichiometric method, a set of independent chemical reactions are specified, and the

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equilibrium concentrations are then calculated by solving for the extent of every reaction. However, when implementing the non-stoichiometric method, no reactions are specified and the concentrations of the gas species are evaluated to minimize the Gibbs energy of the products [5, 6]. Since the non-stoichiometric approach does not need a detailed specification of all the chemical reactions occurring in the reactor, numerous researchers have focused on this method. It is worth mentioning that the authors are only aware of very few published simulation studies on biomass gasification systems using the stoichiometric method [5]. Hence, the objective of this study is to develop a steady state computer model for waste biomass gasifier using ASPEN Plus simulator based on stoichiometric equilibrium method. Then this model is used to evaluate comparatively the gasification performance of two feedstocks of wood chips and mixed paper wastes. The effect of operating parameters of temperature and moisture content (MC) on high heating value (HHV) of produced syngas and cold gas efficiency (CGE) are investigated [7].

2. MATERIALS AND METHODS

A new kinetic free equilibrium model based on stoichiometric approach has been developed for the downdraft air gasifier of waste biomasses by using ASPEN Plus version 10. Penge Robinson equation of state with Boston-Mathias alpha function (PR-BM) was used to estimate all physical properties of the conventional components in the gasification process. This method can be appropriate for hydrocarbons and light gases as nonpolar/mildly polar mixtures and alpha parameter in this approach are temperature dependent variables that can be useful for the correlation of the vapor pressure of pure component when temperature is very high. Furthermore, HCOALGEN and DCOALIGT models were selected for enthalpy and density of biomass and ash which are non-conventional components. MCINCPSD stream comprising three substreams of MIXED, CIPSD and NCPSD class, was also used to define the structure of biomass and ash streams which are not available in Aspen Plus component database. Moreover, the model is based on the following 7 assumptions: (1) The model is at steady state, kinetic free and isothermal. (2) All gases are ideal gases, including hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), steam (H_2O), nitrogen (N_2) and methane (CH_4). (3) Char contains only carbon and ash in solid phase. (4) Tar and other heavy hydrocarbons are not considered. (5) Operation at atmospheric pressure (~ 1 bar). (6) No heat and pressure losses take place in the gasifier. (7) Simulation is based on stoichiometric equilibrium approach and based on reactions in Table 1 [7].

Figure 1 shows the flow chart of waste biomass gasification simulation using ASPEN Plus based on the stoichiometric approach and Table 2 is a brief description of the unit operations of the blocks used in the simulation. The BIOMSS stream was defined as a nonconventional stream and it was created by specifying the elemental and gross compositions of feedstock obtained from proximate and elemental analyses given in Table 3. In the next step, RYIELD, the yield reactor in ASPEN Plus, was brought to simulate the decomposition of the feed. In pyrolysis/decomposition step, the feedstock is converted to volatile materials (VM) and char. VM includes carbon, hydrogen, oxygen and nitrogen; Char is also converted into ash and carbon, by specifying the product distribution based on the proximate and ultimate analysis of the feedstock. The yield of volatiles is equal to the volatile content in the fuel according to the proximate analysis [8-10]. For stoichiometric equilibrium simulation of the combustion and gasification of biomass, REquil reactor was used in which homogeneous and heterogeneous reactions can be defined, simultaneously. However, due to the limitation of ASPEN Plus that each REquil can only contain one heterogeneous reaction, four REquil reactors (RE1-RE4) were considered for 4 heterogeneous reactions of R1, R2, R3, R5 (shown in Table 1).

TABLE 1: THE CONSIDERED REACTIONS IN THE MODEL

R1	$C + 0.5O_2 \rightarrow CO$	Partial combustion
R2	$C + O_2 \rightarrow CO_2$	Complete combustion
R3	$C + H_2O \rightarrow CO + H_2$	Water-gas
R4	$H_2 + 0.5O_2 \rightarrow H_2O$	Hydrogen combustion
R5	$C + 2H_2 \rightarrow CH_4$	Methanation

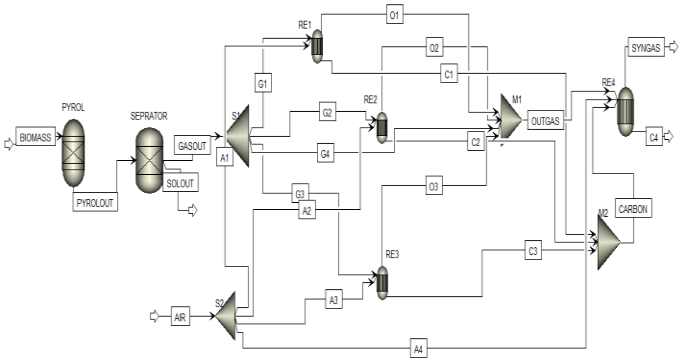

FIGURE 1: FLOW CHART OF WASTE BIOMASS GASIFICATION SIMULATION USING ASPEN PLUS

Two FSplit blocks were used for dividing streams of volatiles and air among reactors of RE1, RE2 and RE3 (for R1, R2 and R3). Then two Mixer blocks were used to mix outlet gasses and unburned carbons from the up and bottom of reactors, respectively; the product streams called OUTGAS and CARBON, respectively. Then, OUTGAS and CARBON streams with the rest of air stream were entered to RE4 for the heterogeneous reaction of R5 and homogenous reaction of R4. Eventually, the product gas called SYNGAS was exited from the up of RE4.

TABLE 2: DESCRIPTION OF ASPEN PLUS UNIT OPERATION BLOCKS USED IN MODEL

ASPEN Plus name	Block name	Description
Ryield	PYROL	Decomposition of non-conventional biomass to conventional components according to its proximate and ultimate analyses
Requil	RE1, RE2, RE3, RE4	Rigorous equilibrium reactor based on stoichiometric approach
Sep	SEPRATOR	Gas separation from ash by specifying split fractions
FSplit	S1, S2	Dividing of gas stream and air stream based on split fractions by S1 & S2, respectively
Mixer	M1, M2	Blending of gasses and carbons into one stream by M1 & M2, respectively

TABLE 3: ULTIMATE AND PROXIMATE ANALYSIS

Feedstocks	Wood chip	Mixed paper waste
Proximate analysis (wt%)		
Moisture	20	8.8
Volatile matter (VM)	80	84.2
Fixed carbon (FC)	18.84	7.5
Ash	1.16	8.3
Elemental analysis (wt%-dry basis)		
C	51.19	47.96
H	6.08	6.60
N	0.2	0.18
O	41.37	36.96

3. VALIDATION

For validating the presented model, the syngas composition obtained from ASPEN simulations were compared with the experimental results of Jayah et al [11]. In their work, rubber wood was used as feedstock in a down draft gasifier operated at atmospheric pressure and gasification temperature of 900 ˚C. Six different air to fuel mass flow rate ratios (AFRs) were considered and the comparisons of CO, H_2, CO_2 and N_2 concentrations are shown in Fig. 2. The deviation of the model results from experimental values is quantified by using statistical parameter RMS. RMS measures how much error there is between two data sets (experimental data and modeling values). Its value close to zero indicates lower error and more reliable model in prediction of results. The maximum RMS error of 1.89 is gained when six sets of experimental data are compared with the corresponding model values for syngas composition. The obtained RMS in this work is good and acceptable because it is not far from zero and also lower than other works in this field. For example Rupesh et al. [12] obtained RMS of 2.8 in comparison of experimental data and modeling values for product gas compositions.

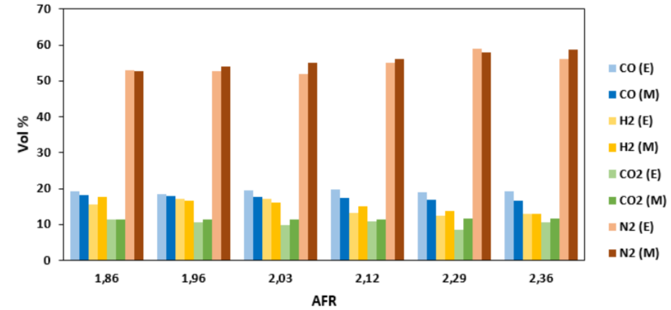

FIGURE 2: COMPARISON OF CO, H_2, CO_2 AND N_2 CONCENTRATIONS BETWEEN STOICHIOMETRIC MODEL (M) AND EXPERIMENTAL MEASUREMENTS (E)

4. RESULTS AND DISCUSSION

The developed model was used to study the gasification performance of two different waste feedstocks of wood chips and mixed paper waste. Then, the effect of gasifier temperature and MC on LHV of produced gas and CGE has been investigated. The LHV of syngas is calculated as [8, 13]:

$$LHV_{syngas}(kj/Nm^3) = 4.2\times(30\times y_{CO}+25.7\times y_{H_2}+85.4\times y_{CH_4}) \qquad (1)$$

where y is the mole fraction of gas pieces in the syngas (dry basis).

The CGE is also calculated by using equation (2) [8, 14]:

$$CGE(\%) = \frac{G_P \times LHV_{syngas}}{HHV_{fuel}} \times 100 \qquad (2)$$

where G_P is the syngas yield that is the volume of total product gas from the gasification per unit weight of fuel in normal conditions (Nm^3 kg fuel-1). HHV_{fuel} is the higher heating value of fuel (MJ kg fuel-1) [15].

$$HHV_{fuel}(Mj/kg) = 0.312\times(FC)+0.1534\times(VM) \qquad (3)$$

According to equation (3), heating value is a function of weight fractions of fixed carbon and volatile matter in the dry and ash-free conditions.

4.1 Effect of temperature and MC on LHV

The effect of gasifier temperature on LHV of syngas for two feedstocks was examined in the window of 500-1500 ˚C, while all the remaining operating conditions were fixed (equivalence ration (ER)=0.4 and MC according to Table 3). As shown in Fig. 3, the increase in temperature results in an increase in the LHV of the syngas until a specific temperature that is called optimum temperature. At very low temperature of 500 ˚C the existing carbon in the biomass is not used completely, so the syngas would be produced at a low yield. At such a low temperature, unburned carbon and methane will remain in the syngas. By increasing the temperature more carbon is oxidized and converted to carbon monoxide in accordance with partial combustion reaction (R1). Methane is also transferred into hydrogen by reverse methanation reaction (R5). At higher temperature, water gas reaction (R3) shifts toward the production of both carbon monoxide and hydrogen. Hence, increasing the gasifier temperature favors hydrogen and carbon monoxide production, which leads to the improvement of heating value of syngas (based on equation (1)). However, at a specific temperature, the yield of H_2 and CO approach a plateau; the onset of this plateau is typically the optimal gasifier temperature for every type of waste stream evaluated here. The optimum operating temperature of the down draft gasifier for wood chips and paper wastes are both around 900 ˚C. LHV values for wood chips and mixed paper wastes at optimum temperatures are about 3.79 and 4.06 MJ Nm^3, respectively.

Wood chips shows lower heating value than paper waste due to relatively lower dry basis mole fraction of CO and hydrogen in the syngas. The production of CO and hydrogen is dependent on the biomass composition and it is clear from the composition of feedstock streams provided in Table 3 that although wood chips have highest percentage of carbon, they include a high amount of moisture. MC indirectly effects on LHV of syngas (Fig. 4). Increasing moisture content strongly degrades the syngas LHV. Because of much higher moisture content in the fuel, the percentage of carbon and hydrogen in wet basis decrease then leads to lower production of carbon monoxide and hydrogen in the syngas.

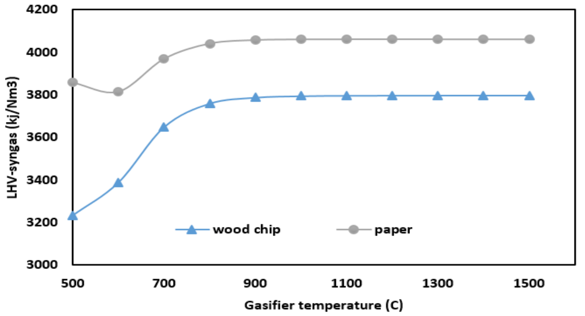

FIGURE 3: EFFECT OF TEMPERATURE ON LHV

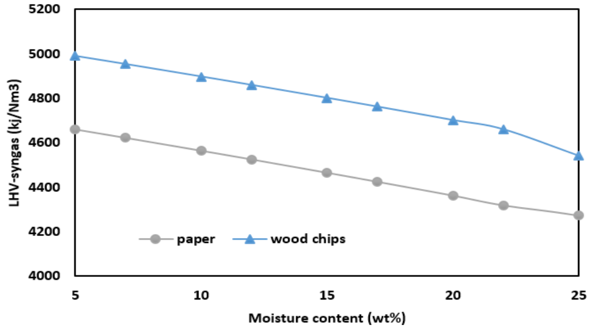

FIGURE 4: EFFECT OF MC ON LHV

4.2 Effect of temperature and MC on CGE

In our model temperature has been varied from 500-1500˚C and the corresponding CGE as the most crucial parameter for economic efficiency evaluation of the gasifier is calculated. The results have been depicted in Fig. 5. Accordance to equation (2), CGE is dependent on different parameters of syngas yield, HHV of fuel and LHV of syngas. Syngas yield and LHV depend on the amount of carbon monoxide, hydrogen and methane in the product syngas and HHV of wood chips and paper wastes were calculated 18.37 and 16.63 MJ kg^{-1}, respectively. Mixed paper waste shows highest CGE (70.5%) at temperature of 900 ˚C while for wood chips CGE is maximum around 60%. Fig. 6 shows that increasing MC reduces the value of CGE, stemming from the reduction of LHV (Fig. 4). For the two waste biomass streams, the amount of CGE is under 65% as long as ER is more than 15%. It follows that MC should be kept below this level.

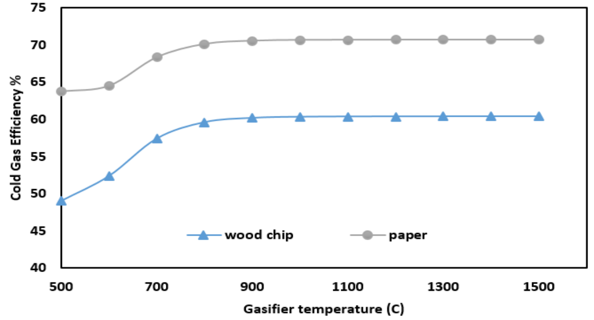

FIGURE 5: EFFECT OF TEMPERATURE ON CGE

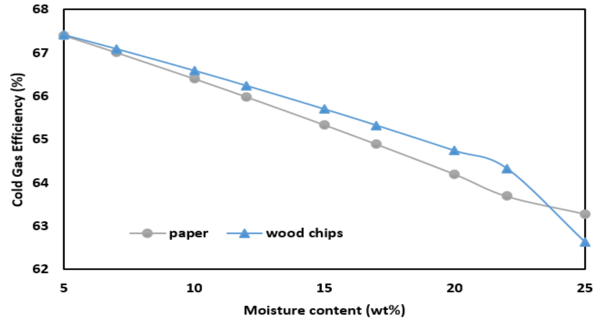

FIGURE 6: EFFECT OF MC ON CGE

5. CONCLUSION

A new steady state model simulating downdraft waste biomass gasification was developed using Aspen Plus based on stoichiometric equilibrium approach, modified with restricted chemical reactions equilibrium in the gasification reduction zone. The model was successfully validated with experimental data of downdraft rubber wood gasification, with good agreement on the main syngas compositions. Subsequently the effect of gasification temperature and biomass moisture content on HHV of syngas and CGE was investigated. Increasing temperature improves the gasifier performance, it increases the production of CO and H_2 which leads to higher LHV and CGE. However, high moisture content reduces gasifier performance and results in low CGE. In order to achieve optimal gasification performance, it was recommended that the gasification temperature should be around 800-1000 °C and the biomass moisture content should be less than 15%.

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