

Simulation of rice straw gasification in bubbling bed reactor using ASPEN PLUS

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Abstract: The global dependence on fossil fuels and the environmental effects of them are some of the factors that urge research on using biomass sources. Gasification is a process which converts carbonaceous materials into syngas. In this study, a bubbling bed gasification model is developed for the gasification of rice straw as a feedstock by using ASPEN PLUS. Thermodynamic equilibrium model which is based on the minimization of the Gibbs free energy of the system was used. The results of gasification in bubbling bed gasifier were verified by using data from literature. The gasifier temperature and steam flow rate are the most important parameters that influence the chemical composition of the syngas for the rice straw gasification in bubbling bed gasifier. Increasing steam-to-biomass ratio enhances H_2 , CH_4 and CO production, while decreases CO_2 . Furthermore, results showed that the developed bubbling bed gasifier model can be robust model, if gasifier temperature is selected within the 500–1000 °C temperature range.

Keywords: Rice Straw, Bubbling Bed Gasifier, Biomass Gasification, Aspen Plus, Simulation.

I. INTRODUCTION

Increasing global energy demand and environmental worries, researchers to shift fossil fuels with clean energy resources. In Europe, biomass is recently used as renewable energy sources for electricity generation, biofuels production for transport, useful heat generation especially [1]. Biomass as a renewable energy source, which includes variety of waste materials from plants or animals, reduces gas emissions. After biomass utilization process, CO_2 released to environment but biomass absorbs CO_2 from the environment during photosynthesis. Because of this cycle, biomass carbon dioxide becomes neutral. Biomass types have many differences according to their chemical and physical properties. Elemental composition, moisture content, ash and volatile matter content are the main properties of biomass [2]. Heating value is one of the most important parameter that effects the biomass usage. Lower heating value of biomass provides effective heat and mass transfer thus system is worked with more energy efficient and higher performance.

Gasification process has been identified as a promising method to convert biomass source into fuel gas due to its low cost and high fuel gas production efficiency [3,4]. Biomass

gasification aims to convert solid biomass into a syngas which mainly consists of hydrogen (H_2), methane (CH_4), carbonmonoxide (CO), carbondioxide (CO_2), water (H_2O) and trace amount of higher hydrocarbons. Gasification process is consist of four parts, biomass drying, pyrolysis, gasification and combustion. Several chemical reactions take place under steam, oxygen and/or air atmosphere in the gasification process. Steam gasification increases the hydrogen yield of product gas and also provides higher standard synthesis gas [5]. The main products of gasification such as syngas, tar, char and their properties and amount depend on the operational conditions, gasification agent and elemental and physical properties of feedstock [6,7]. Depending on the process, produced gas can be used to create diesel or gasoline, methanol for the chemical industry, hydrogen fuel and fertilizers by processing ammonia [8].

Gasification is also preferred for the lower pollutant effects and more efficient heat and power generation [9,10]. On the other hand, gasification requires to develop modern gasifiers to prevent problems regarding biomass tar production, product gas impurities [11,12].

Gasifiers are the reactor type where gasification process occurs [13]. Gasifier types includes fluidized bed, fixed bed,

and entrained flow are chosen with respect to biomass properties such as size, shape, ash content, amount, moisture content and operation terms [14]. Fluidized bed gasifiers have fluidization principle that bed material and fuel act like fluid [15]. Silica is the mostly used inert bed material for fluidized bed gasifiers, although other materials such as sand, dolomite, glass beads and olivine show catalytic features and reduce tar problems. Fluidized bed reactors divide into two categories according to their technics of fluidization; bubbling fluidized and circulating fluidized [14]. The main aim of the fluidized bed gasifier is to improve heat and mass transfer among the fuel particles and gasification agent. The bubbling bed gasifier has many advantages in terms of high carbon conversion efficiency, homogenous temperature distribution and flexibility regarding feedstock type and size. Bubbling bed gasifiers has complicated process so are influenced from many properties such as steam/fuel ratio, reaction temperature and equivalent ratio. All of these properties effect directly chemical composition of the syngas in bubbling bed gasifier [16,17].

Modeling based methods provide alternative and economical ways to the designing and optimization of complicated systems such as gasification [18]. Aspen Plus is an useful program to optimize system parameters. It is used to develop model which is more cost effective than experimental studies. Many researchers are used Aspen Plus for modelling of gasification process. Han et al. [19] developed an air-gasification model using Aspen Plus and investigated the effect of main parameters in biomass gasification on the quality of produced gas based on minimizing Gibbs free energy. Rupesh et al. [20] found that H_2 reached the maximum value (H_2 volume percentage of 31.17%) at steam/biomass ratio of 1.0, ER of 0.25 and gasification temperature of 900 K using Aspen Plus. Nikoo and Mahinpey [21] carried out simulation of gasification based on bed hydrodynamics and reaction kinetics using Aspen Plus. Lan et al. [22] developed an integrated biomass gasification via Aspen Plus and showed the effect of the main parameters for power generation.

The main purpose of this study is to provide a general model for the type of bubbling bed gasifier by using Aspen Plus program. The proposed model was validated with the experimental data sets obtained from the literature. To investigate the impact of operation parameters including gasification temperature and steam flow rate on the composition, heating value and exergy of syngas from bubbling bed rice straw gasifier, the sensitivity analysis was applied.

II. MATERIALS AND METHODS

In this part, biomass sample properties, block diagram of bubbling bed gasifier, process assumptions and definition of the blocks used in the Aspen Plus software is reviewed.

A. Materials

Biomass characteristics are the main factors affecting the heating value, composition and exergy of syngas from the developed Aspen model, therefore, they are detailed in this study. The rice straw used in this study was supplied by the local suppliers from north of Turkey. Rice straw is an organic waste material which is result of rice production. Rice residues causes environmental pollution especially in places where production take place on large scale.

TABLE I. PROXIMATE AND ULTIMATE ANALYSIS OF RICE STRAW

Proximate Analysis (wt%)	Volatile Matter	68.52
	Ash	14.34
	Moisture	2.55
	Fixed Carbon	14.59
Ultimate Analysis (wt%)	Sulfur	2.06
	Oxygen	53.66
	Nitrogen	0.79
	Hydrogen	5.13
	Carbon	38.36

Ultimate and proximate analysis results were conducted according to ASTM Standard D5373-2 and ASTM Standard D5142-04, respectively. The results are identified in Table 1. Mass percentage of the oxygen content was determined by the difference in a dry ash free basis content, using Eq. 1.

$$O(\%) = 100 - (N + C + H + S) \quad (1)$$

B. Model Description

Bubbling fluidized bed gasifier model has been studied according to principles of chemical, energy, and mass balance by using Aspen Plus simulation. Gasification model flowsheet is built by using different blocks in the Aspen Plus software. Stream informations and physical property method is inserted to system to conduct simulation. The developed model in this study is based on the principle of minimization of Gibbs free energy to reach equilibrium. Syngas production process under steam atmosphere includes several process which are low temperature pyrolysis, high temperature pyrolysis and gasification, respectively. Pyrolysis is a thermochemical

decomposition, which can be applied to any organic (carbon-based) product. Biomass was defined as a non-conventional component for Aspen plus BIOMASS stream, the low temperature pyrolysis converts the biomass into its conventional components. High temperature pyrolysis is the first step for the conversion of rice straw to syngas. After pyrolysis steps, gasification has been simulated at between 500-1000°C to determine the optimum gasification temperature. In the simulation of gasification process, the following assumptions were considered:

- Model operates in steady-state conditions
- It is an isothermal process
- There is no pressure decrease in the gasification parts
- All gases behave ideally
- Ash is inert and is not involved in reactions which is occurred in gasification process.
- Bio-char conversion is 100%

There is not a particular reactor or block to define the gasifier, in Aspen Plus simulation. Combination of different block was used to represent the gasification process. The reactor is divided into three sections as Decomp, Gasif1, Gasif2 as shown in Fig. 1.

TABLE II. OPERATION BLOCKS IN ASPEN PLUS MODEL

<i>ID</i>	<i>Block Type</i>	<i>Description</i>
DECOMP	RYIELD	Biomass converts into conventional components
GASIF1, GASIF2	RGIBBS	Simulates the gasification reactions by using Gibbs free energy minimization
SPLITTER	FSPLIT	Dispenses steam into Gibbs reactors
SEP1, SEP2	SEP	SEP1 block performs the separation of certain amounts of CH ₄ and CO ₂ . SEP2 block separates water, H ₂ S and ash from producer gas.

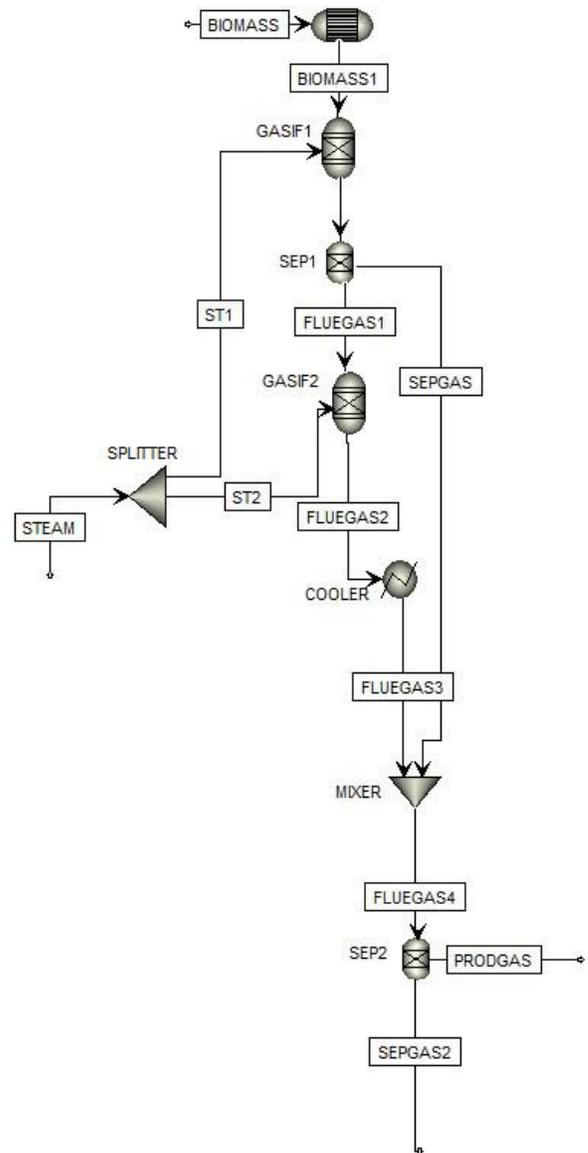


Fig. 1. Flow Sheet of Rice Straw Gasification.

Biomass is fed into to Decomp reactor which is identified RYIELD in Aspen Plus. In Decomp reactor, form of rice straw was changed from nonconventional to conventional components which are oxygen, hydrogen, nitrogen, carbon, ash and sulfur according to the its proximate and ultimate analysis. Steam is divided into two streams via FSplit block which was named as Splitter to create steam atmosphere in the Gasif1 and Gasif2. RGIBBS block was used to simulate the pyrolysis part where is occurred in Gasif1. Sep1 block was placed to perform the separation of certain amounts of CH₄ and CO₂ before gasification step. Gasification reactions is occurred in the Gasif2 block which is represented also RGIBBS reactor. Flugas2 which is produced by gasification process is sent to Cooler block to decrease the product gas temperature. Flugas3

is mixed with Sepgas which is coming from Sep1 block via Mixer. Block Sep2 simulates the removal of water, H₂S and ash. Syngas is obtained water and ash free form, it is generally consist of methane, hydrogen, carbonmonoxide and carbon dioxide.

Biomass type, operational conditions and gasification agent can affect the gasification reactions. The moisture from rice straw affects the equilibrium of chemical reaction and involves in gasification reactions such as steam methane reforming reaction, water gas shift reaction, water gas reaction. Medium molecules decompose into the smaller molecules such as carbon monoxide, methane, carbon dioxide and hydrogen (Eq. 9,10). If the residence time during the reaction is not long enough to decomposed for medium molecules, they will formed as tars and oils and go to oxidation zone. Pyrolysis region products reacts with the gasfying agent for production of smaller molecules. In the reduction region, water gas reaction (Eq. 7), water gas shift reaction (Eq. 4), methanation reaction (Eq. 2) and steam methane reforming Eq. (8) Boudouard reaction (Eq. 5) occur because of inadequate oxygen in the high temperature region. The reactions in bubbling fluidized bed gasifier are represented in Table 2.

TABLE III. GASIFICATION REACTIONS

$C + 2H_2 = CH_4$ (hydrogasification reaction)	(2)
$C + 1/2O_2 = CO$ (partial oxidation reaction)	(3)
$CO + H_2O = CO_2 + H_2$ (water gas shift reaction)	(4)
$C + CO_2 = 2CO$ (Boudouard reaction)	(5)
$H_2 + S \rightarrow H_2S$	(6)
$C + H_2O = CO + H_2$ (water gas reaction)	(7)
$CH_4 + H_2O = CO + 3H_2$ (steam reforming reaction)	(8)
$C + O_2 = CO_2$ (complete oxidation reaction)	(9)
$H_2 + 0.5O_2 = H_2O$ (hydrogen oxidation)	(10)

III. RESULTS AND DISCUSSIONS

A. Model Validation Results

Experimental data sets from the literature have been used to validate and create the appropriate model for bubbling fluidized bed gasifier. Two different data sets from literature [23, 24] have been chosen for the validation of developed model. The simulation was carried out with the same operational conditions from literature as seen on Table 3. In the first one, wood pellet was chosen as feedstock, gasification temperature is 800°C and air is gasifying agent, air and biomass flow rate is represent in Table 3. Second experimental data from literature is also shown in Table 3, tire sample is feedstock, gasifier temperature is 770°C and steam is used as gasfying agent.

TABLE IV. EXPERIMENTAL CONDITIONS AND VALIDATION RESULTS OF AIR AGENT GASIFICATION [23] AND STEAM AGENT GASIFICATION [24]

1		
Wood Pellet	Biomass(kg/h)	34
Gasifier - 800°C	Air(Nm ³ /h)	37
Gas Composition	1	Model(%)
H₂	14.5	15.67
CO₂	16	16.44
CO	13.8	13.91
CH₄	4	9.09
2		
Tire Sample	Biomass(kg/h)	0.876
Gasifier - 770°C	Steam(kg/h)	0.331
Gas Composition	1	Model(%)
H₂	48.81	47.87
CO₂	3.30	3.56
CO	3.89	3.2
CH₄	26.37	14.3

As it can be seen in Table 3, H₂, CO, CO₂ compositions are very similar in the experimental and the developed model. However, CH₄ composition from the air gasification data from literature, it is quite different compared to other gas compositions because the Aspen Plus model works basis of thermodynamic equilibrium so fuel residence time in the gasifier would be different in the model and experimental study. From the validation results of the developed model, we can obtain that in spite of there are some differences in validation results, these deviations are not that important, the simulation model give a quite good idea of the product gas composition. It is the main goal of this model.

B. Model Results

After model validation, a series of bubbling bed simulation were conducted in order to observe the effects of steam flowrate and temperature on the syngas composition and its LHV and exergy value. Sensitivity analysis was used to investigate effect of temperature and steam flow rate on the syngas composition, LHV of syngas and exergy value of syngas.

1) Effect of Gasification Temperature

a) *Syngas Composition:* The plot of selected syngas composition (CO₂, CH₄, H₂ and CO) on a dry basis as a function of temperature have been shown in Fig. 2. The model performed sensitivity analysis for the bubbling fluidized bed gasifier for the temperature between 500–1000 °C.

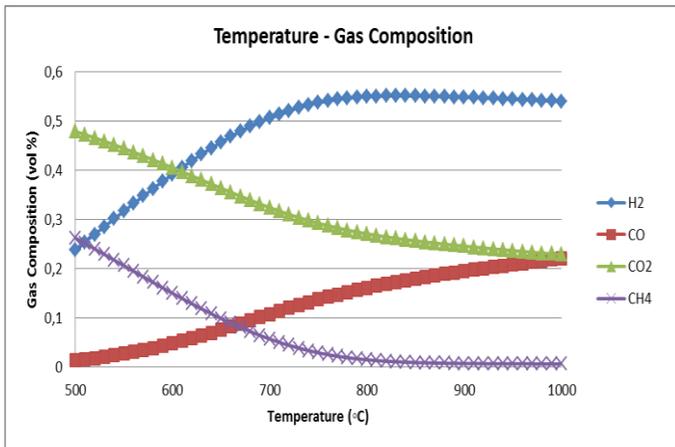


Fig. 2. Effect of gasification temperature on syngas composition.

Endothermic char gasification and steam reforming reactions play a significant role for the increase in H₂ and CO molar fractions. At lower gasification temperatures, which is below the 700 °C, CO and H₂ molar fraction increased with the temperature change. However, at relatively high temperatures, the endothermic reactions are reinforced through the temperature change, which proves the feasibility of Le-Chatelier's principle [25]. With respect to Boudouard reaction, while the gasifier temperature increasing, mole fraction of CO₂ decreases and CO increases. H₂ mole fraction changes between %23,8 and %55.1, it reaches to maximum value at 840°C. Gas composition change is negligible between the gasification temperature 850-1000 C. An increment in gasification temperature could be rise the operational charge. CO is converted to H₂ via water gas shift reactions and a faster growth rate is observed in H₂ than CO. CH₄ concentration decreased, while H₂ and CO concentration increased because of the methanation reaction. CO₂ molar fraction change showed a similar tendency with the change of CH₄ molar fraction. Former studies in the literature shows the similar results for gasification process in bubbling fluidized bed gasifier. For example, Skoulou et al.[26] found that, the mole fractions of H₂ and CO increased and mole fractions of CO₂ and CH₄ decreased with increasing temperature. Begum et al.[27] also studied effect of gasification temperature on syngas composition and found same results for the municipal solid waste (MSW) gasification process.

b) *Lower Heating Value (LHV)*: LHV of syngas is a physical property which is a very important parameter for the energy evaluation of gasification process. Lower Heating Value (LHV) of syngas depends on the combustible properties of components. Temperature effects the mass basis syngas LHV positively, Fig. 3 shows the behavior of syngas LHV versus temperature.

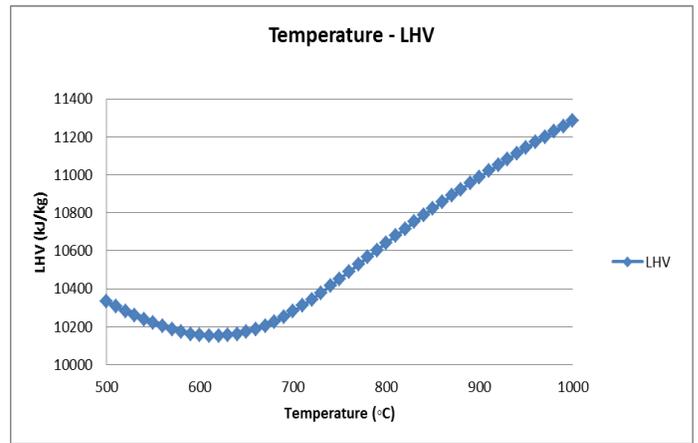


Fig. 3. Effect of gasification temperature to syngas LHV.

Among the all combustible component in syngas, CH₄ is the more effective component than H₂ and CO for the syngas LHV. LHV decreases with temperature increases between the temperature 500-620°C because of the decreasing of CH₄ mole fraction. Then H₂ and CO mole fractions, which favor LHV, rise up fairly with increasing of temperature results the enhance in Fig. 3.

c) *Exergy*: Exergy is the helpful tool for performance analysis of systems. The increase in temperature promote the exergy value of the syngas composition because of the enhancement of chemical exergy value through H₂ and CO production. Moreover, physical exergy with the temperature increase also assist the exergy value of syngas composition. On the other hand, excessive temperature change influences the gasification reactions results decreasing exergy value. According to the sensitivity analysis in this study, maximum exergy has been obtained at the 820°C as seen on Fig. 4.

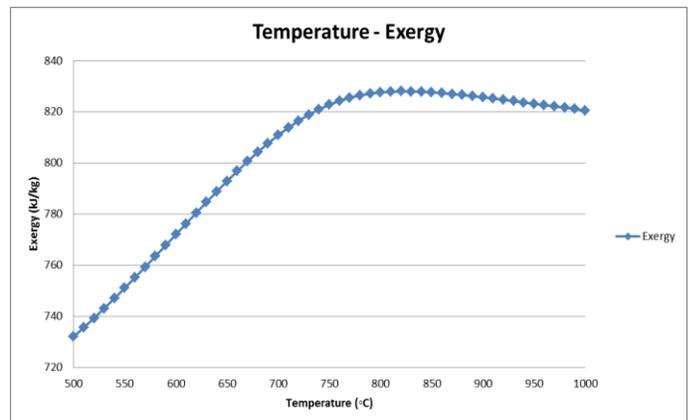


Fig. 4. Effect of gasification temperature to syngas exergy.

2) Effect of Steam Flow Rate

a) *Syngas Composition*: To observe the effect of steam flow rate on syngas composition, a sensitivity analysis was

conducted at steam flow rates of 7 and 60 kg/h. Fig. 5 shows the variation of syngas composition (CO_2 , CO and H_2) at different steam flow rates. The steam flow rate remarkably influenced the composition of syngas generation during steam gasification, and increasing of steam flow rate shifts directions of reactions (steam-methane reforming and water-gas shift) to Hydrogen production. H_2 mole fraction increased in the syngas.

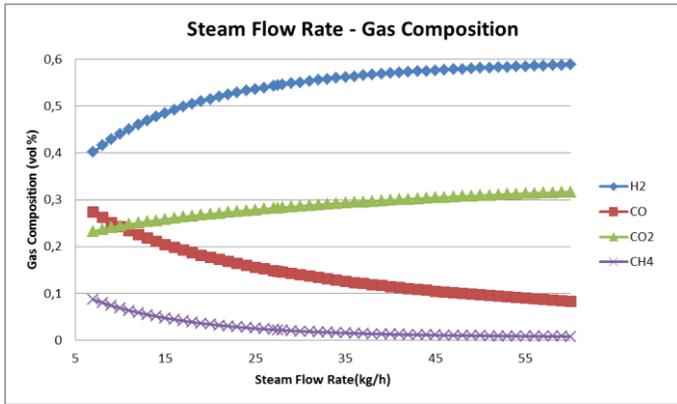


Fig. 5. Effect of steam flow rate to gas composition.

Complete combustion reaction occurs more than partial combustion reaction with increasing amount of gasifying agent. Thus, higher steam flow rate decreases the mole fraction of CO from %27 to %8 and increases the mole fraction of CO_2 from %23 to %31 in the syngas. CH_4 mole fraction decreased from %8 to %0.08 because of steam-methane reforming reaction shifts to product side with increasing steam flow rate. Therefore, methane mole fraction decreases and H_2 mole fraction increases via steam methane reforming reaction.

b) *Lower Heating Value:* LHV is expressed the energy contents. Components in the syngas have different energy content. The selectivity of the gasification reactions varies with steam flow rate, thus affecting the composition and LHV of syngas. Fig. 6 presents the LHV at different steam flow rate.

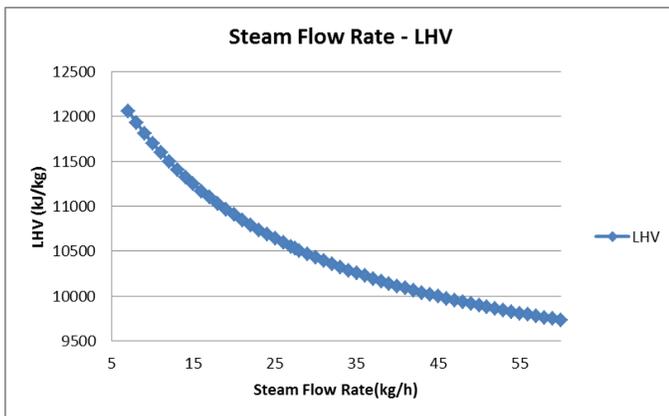


Fig. 6. Effect of steam flow rate to syngas LHV.

In the Fig. 6, it can be seen that LHV decreases with the increase of steam flow rate. The increment in steam flow rate complete oxidations includes CO_2 formation. As a result of complete oxidation reaction, CO_2 amount increase and CO amount decreased and combustible component amounts decreased significantly. CH_4 is the important combustible component and influences the lower heating value of syngas. As seen on Fig. 5 CH_4 composition in syngas and LHV value of syngas shows decreasing trend with temperature increases. For this reason, LHV of syngas has a decreasing tendency between 12000 and 9500 kJ/kg.

c) *Exergy:* Exergy analysis is used to performance evaluation of the gasification process. Fig. 7 shows the exergy value from rice straw gasification under steam atmosphere at different steam flow rate.

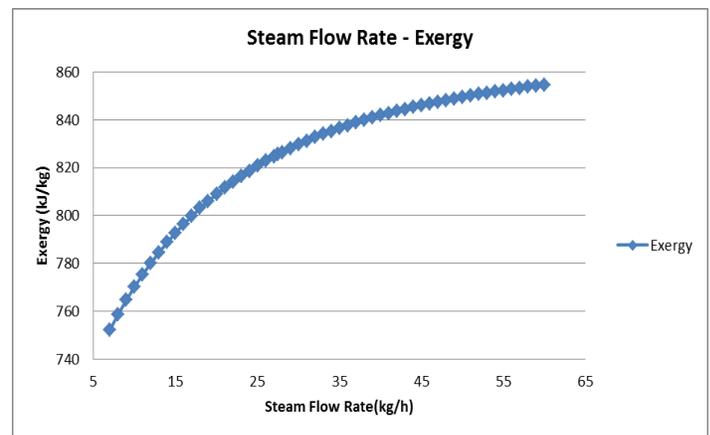


Fig. 7. Effect of steam flow rate to syngas exergy.

When the steam flow rate was increased from 7 to 60 kg/h as seen on Fig. 7, the exergy value increased. The increase in steam flow rate favoring hydrogen production via gasification reactions includes hydrocarbon cracking reactions, water gas reaction (Eq.7), methane steam reforming reaction (Eq.8), water gas shift reaction (Eq.4), and steam gasification of condensable volatiles under steam atmosphere. Therefore, the results show that the exergy value from steam gasification of rice straw is mainly determined by the chemical exergy of biomass because of the hydrogen production.

IV. CONCLUSION

With respect to the objectives of this study, we conclude that:

- Bubbling fluidized bed gasifier model successfully validated with two experimental data sets.
- System was designed to utilize the biomass as feedstock that produced synthesis gas.

- We examined the effect of different working parameters for bubbling fluidized bed gasifier using sensitivity analysis.
- Temperature and steam flow rate showed considerable effects on the composition of syngas.
- LHV and exergy value of syngas is strongly influenced by the operation temperature.
- H₂ and CO content increased slightly with the increase of the temperature, to be more specific the content of H₂ increased by about 33% from 500°C to 820°C, while the content of CO increased by about 15% from 500°C to 820°C.
- LHV decreased while temperature increase between 500°C to 620°C; increasing of temperature from 620 to 1000°C, LHV was shown an increasing trend from 10154 to 11285 kJ/kg.
- Increment in temperature, exergy value increased and reached the maximum value at the 820°C.
- Effect of steam flow rate is observed on the syngas lower heating and exergy value.
- With the addition of steam, the content of H₂ increased significantly, from 40% to 58%. Molar fraction of CO decreased and molar fraction of CO₂ increased between 27% to 8% and 23% to 31%, respectively.
- LHV of syngas changed between 12000 and 9500 kJ/kg while steam flow rate increased from 7 to 60 kJ/kg.
- Increasing of steam flow rate, the exergy value of syngas increased from 752 to 854 kJ/kg. Exergy value and molar fraction of H₂ of produced gas show same trend with temperature change.
- LHV and exergy value of syngas have been effected by increment of H₂ and CO production.
- For future study, the developed bubbling bed gasifier model will be integrated with a gas turbine, steam turbine or high temperature fuel cell stack.

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