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Simulation of Biomass Gasification Model for Syngas Production from Wood Residue and Food Wastes

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ABSTRACT

Utilizing Aspen Plus, a biomass gasification model has been developed for syngas production from wood residue and food wastes, while steam is used as the gasifying agent. The framework uses the constrained equilibrium approach to Gibbs free energy reduction. This research aimed to examine how essential variables such as reactor temperature and the ratio of steam flow rate with respect to biomass feed flow rate to the gasifier affected the concentration of syngas composition and H_2/CO ratio of the syngas. Biomass is converted to syngas through pretreatment, high-temperature gasification, and impurity removal for versatile energy and chemical applications. Simulations were performed for different biomass feedstocks, specifically wood residues (WR) and food wastes (FW), to predict their syngas compositions like hydrogen (H_2), carbon monoxide (CO), carbon-di-oxide (CO_2), and methane (CH_4) concentrations. Based on this model, the effects of the reactor temperature of the gasifier and steam flow rate concerning the feed flow on syngas yield and lower heating value (LHV) were thoroughly investigated. The mass flow rate, molar fraction, molar flow rate, syngas yield, and LHV were analyzed for WR and FW. The results indicated that the syngas yield was approximately 1.2 Nm^3/kg for WR and 1.3 Nm^3/kg for FW, with corresponding LHV values around 11 MJ/kg and 12 MJ/kg, respectively. The effects of varying gasification temperature at a fixed S/B ratio (SBR) of 0.6 and adjusting the SBR at a gasifier reactor temperature of 700ºC were considered. The H_2/CO molar ratio was determined to optimize with shift reaction, yielding a product gas composition with an H_2/CO ratio of about 1.9 for WR and 1.3 for FW. These findings highlight the potential for optimizing gasification parameters tailored to specific biomass feedstocks to enhance syngas production efficiency and quality.

Keywords: Biomass Gasification, Aspen Plus, Syngas Production, Gasification Temperature, Steam-to-Biomass Ratio

1. Introduction

In this present era of energy crisis and climate change due to the rapid burning of fossil fuels, there is an urgent need for alternative sources of energy. Biomass is a clean, renewable energy source that can be a replacement for fossil fuels in the near future [1]. A thermochemical system that produces syngas from carbon-based material is generally known as gasification. The production of syngas may be broken down into four distinct phases: drying the biomass, pyrolysis, gasification, and combustion. High-quality syngas often possesses several features, including a low nitrogen (N_2) content, a high hydrogen (H_2) concentration, and a high heating value, represented by HHV [2]. Steam gasification is often used to enhance its intrinsic value, as it raises the amount of hydrogen present in the mixture. It also has several other benefits, including increased heating value, an adequate dwell time, and efficient soot and carbon removal [3]. Fluidized bed gasifiers (FBG) are particularly beneficial for converting biomass. It may provide excellent energy transfer and high fuel flexibility among the gas and solid stages. They are especially appropriate for biomass gasification since they also maintain a consistent temperature, which is more straightforward to regulate [4]. Aspen Plus is a popular simulation program for simulating biomass gasification operations. It makes it possible to forecast the composition of syngas based on predetermined biomass feedstocks, gasification parameters, and gasifying agent selection [2]. An efficient internal rotating fluidized-bed gasifier was investigated by Doherty et al. [5]. They utilized the Aspen Plus, which worked effectively at an industrial scale with an 8 MW fuel input. The restricted equilibrium model has been confirmed using actual plant data. Air-to-fuel ratio, moisture content, S/B ratio, reactor temperature (gasifier), and steam temperatures were among the operational parameters that were studied. The findings demonstrated a tight match between the published experimental data and the expected heating value, cold gas efficiency, and syngas composition. Sreejith et al. [6] developed another equilibrium model for biomass steam gasification using the Aspen Plus simulator. The model assumed carbon would be completely turned into gases and no tar would form. The effects on decreased heating value, combustible gas yield, and product gas composition were studied in a sensitive analysis. Using the simulation tools listed above, Warnecke et al. [4] developed a model for hydrogen production from wood in gasifiers. Experimental data was used to validate the present model, where pine wood was used and gasified in a small-scale FBG. The investigation analyzed the relationship between temperature and the

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dimension of biomass particles, and the amount of steam to biomass affected the composition of resulting gas and how well it converted carbon. Tavakoli et al. [7] optimized hydrogen production from biomass air-steam gasification using sewage sludge via Aspen Plus simulations and multi-objective methods, achieving reduced CO_2 emissions and a hydrogen cost of 1.5 €/kg. Padova et al. [8] modeled biomass gasification in fluidized bed reactors integrated with high-temperature electrolysis for substitute natural gas (SNG) production. Their process achieved 71.4% efficiency through thermal integration, leveraging electrolysis by-products and optimized operating conditions for enhanced hydrogen production and SNG synthesis.

Aspen Plus simulation models for biomass gasification have been established, although more research is needed on syngas production from biomass sources. This study creates a stable design model of biomass gasification and syngas production utilizing constrained equilibrium reactor shift reactions in Aspen Plus to estimate syngas composition from various reliable biomasses. This research has used food waste and wood residue to assess the model. Therefore, this work details the modeling techniques employed in developing a framework for simulating the gasification operation, including H_2S formation in the stoichiometric reactor and gasification reaction in a restricted equilibrium reactor, with the reactions conducted at specified temperatures. In this study analyzes how gasifier reactor temperature and S/B ratio impact syngas composition and H_2/CO ratio of the product gas. Finally, it predicts the reduced heating value and syngas production of the product gas composition. Published data from a previous experiment on small-scale fluidized bed gasifiers verified the modeling results.

2. Biomass to Syngas Production Process

The biomass-to-syngas production process involves converting biomass like agricultural residues and wood into syngas, a mixture of hydrogen, carbon monoxide (CO), and carbon dioxide (CO_2), through a series of steps. First, the biomass undergoes pretreatment to optimize particle size and moisture content. It then enters a gasification reactor, partially oxidized at high temperatures (700–1600°C) with a controlled amount of oxygen (O_2) or air. Syngas with specific properties can be produced using a variety of gasifiers. The resulting syngas contains impurities like tar, sulfur compounds, and particulates, which are removed through cleaning and conditioning, including filtration, scrubbing, and tar cracking. The final product, syngas, has versatile applications, including power generation, fuel synthesis, and chemical production, making it a valuable intermediate in sustainable energy and materials industries.

3. Aspen Plus Modeling

Biomass gasification with restricted equilibrium reactor has been modeled using Aspen Plus for syngas yielding. Fig.1 depicts the complete modeling process. The following steps were undertaken for the simulation setup:

i. Specifying the Stream Class: The stream class was first defined to categorize the process streams.
ii. Selecting the Property Method: The appropriate property method was chosen from the available options, which aligns with the system characteristics.
iii. System Component Specification: Components were specified and extracted from the database, followed by recognizing standard and non-standard elements relevant to the procedure.
iv. Tailoring the Process Flow-Sheet: The design flow-sheet was then developed by implementing operation blocks and establishing connections between material and energy streams.
v. Feed Stream Specification: Finally, the feed streams were specified, detailing flow rate, composition, and thermodynamic properties or conditions.

The following assumptions are followed to model the process in this study

i. The biomass feed rate is 1000 kg/hr, with 150°C and 1 bar of steam delivered.
ii. The process operates under steady-state and isothermal conditions.
iii. The gasifier maintains uniform pressure and temperature throughout.
iv. The operation occurs at approximately atmospheric pressure (~1 bar).
v. There are no drop of heat or pressure losses within the gasification unit.
vi. The production of tar is neglected, with all sulfur-bound fuel is assumed to be converted into H_2S [2].
vii. No unconverted carbon is present in the output.
viii. The char is believed to be made up entirely of ash and carbon.
ix. Drying and pyrolysis are considered to be instantaneous processes [2].
x. All gases involved are treated as ideal gases.
xi. The product stream consists of H_2, CO, CO_2, CH_4, N_2, H_2O, and H_2S.
xii. The gases use the Boston-Mathias (PR-BM) modification property approach by the Peng-Robinson assumption of condition. [2].

Table 1 lists this investigation's composition of food waste and wood residue. The adequate dwell time in the reactor is a well-known characteristic that makes it difficult for the actual gasification process to establish chemical equilibrium. A considerable deviation has been observed between the predicted and experimental values for the product gas composition while developing the stoichiometric equilibrium model [3]. Better outcomes, however, could be obtained if the restricted equilibrium approach is used in the gasifier reactor model [2]. The equilibrium reactor utilized in this model inside the confined chemical equilibrium serves as the foundation for the model used in this investigation. The "restricted chemical equilibrium with specified temperature method of reactions in the reactor chamber" calculation option also sets the reactions with zero temperature. At the reactor's specified temperature, the reactor block calculates the chemical stability rate for every process by specifying the zero-temperature approach and, therefore, giving the equilibrium gas composition. Eq. (1-9) included in Table 2 present the reactions inside the gasifier, modeled as an RGIBBS reactor. Due to the limitations of heat transfer and fluid dynamics, the substance deposition and catalyst removal are taken into consideration in this procedure. This design uses the Peng-Robinson equilibrium of state, enhanced by the Boston-Mathias amendment (PR-BM), to assess the thermodynamic traits of conventional components.

Table 1 Proximate & Ultimate Analysis of Feedstocks

Feedstock & Composition	Food Waste [9]	Wood Residue [10]
Ultimate analysis (wt.%, dry)		
C	56.65	50.08
H	8.76	6.70
O	23.54	42.51
N	3.95	0.16
S	0.19	0.20
Proximate analysis (wt.%, dry)		
Moisture Content	29.3	5.01
Volatile Matters	72.41	81.81
Fixed Carbon	20.68	17.83
Ash	6.91	0.36

Table 2 Reactions Used in the model [11]

SL No.	Reaction Scheme	Reaction Name	Heat Rejection (KJ/mol)
1	$C+O_2 \rightarrow CO_2$	Carbon Combustion	-393.0
2	$C+0.5O_2 \rightarrow CO$	Carbon Partial Oxidation	-112.0
3	$C+CO_2 \rightarrow 2CO$	Boudouard Reaction	+172.0
4	$C+H_2O \rightarrow CO+H_2$	Boudouard Reaction	+131.0
5	$CO+H_2O \rightarrow CO_2+H_2$	Water Gas Shift Reaction	-41.0
6	$C+2H_2 \rightarrow CH_4$	Methanation Of Carbon	-74.0
7	$H_2+0.5O_2 \rightarrow H_2O$	Hydrogen Partial Combustion	-242.0
8	$CH_4+H_2O \rightarrow CO+3H_2$	Steam Reforming of Methane	+206.0
9	$H_2+S \rightarrow H_2S$	H_2S Formation	-20.2

3.1 Modeling of Biomass Gasification utilizing Aspen Plus

Table 2 displays the reactions involved in this model. 1000 kg/hr had been selected as the overall flow rate. As the foundation for the FEED streams, individuals in Fig. 1 were deemed unconventional streams. The characteristics of biomass components have been introduced to the streams as the final and most accurate analysis. Biomass streams approach the yield reactor in the Decom block, where the decomposition process yields the conventional components, including C, H_2, O_2, N_2, S, and H_2O, as steam and ash [12, 13]. The yield allocation to the Decom reactor block has been set based on the final biomass study. The yield distribution determines the mass flow of each product in the R-FD, the Decom block's outflow stream. The component attributes of ash were specified as unconventional, with a hundred percent of the ash set for both the analyses. Ash is considered a non-conventional component. Ash and carbon char are separated in Separator1, and another stream is named R-FD2, consisting of the remaining composition of gases. The R-FD stream travels to the separator column. Because of the quantity of fixed carbon and the ash, the char split ratio is assigned to a value of unity. Then the R-FD2 proceeds to the stoichiometric reactor named in modeling as STOIC, where all the sulfur transforms to the H_2S according to Eq. 9. Any errors arising from this assumption are insignificant because of the fuel's low sulfur level [10, 12, 14]. C, H_2, O_2, N_2, H_2O, and H_2S are all present in the R-FD3 outlet from the stoichiometric reactor, sent to the separator column as considered Separator2 in this modeling. The primary fuel stream, R-FD4, which is composed of C, H_2, O_2, N_2, and H_2O, is sent to the reactor, named gasifier, while the H_2S gas is separated here as the stream HYSUL.

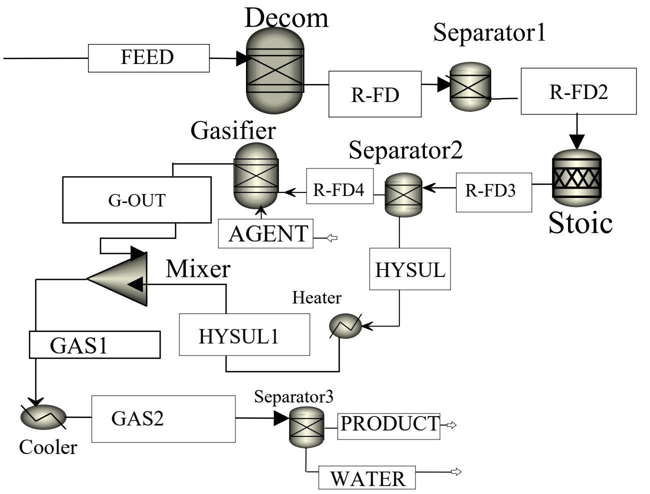

Fig.1 Modeling of biomass gasification utilizing Aspen Plus

Gasification occurs in the gasifier reactor when steam is injected as a stream. Agents use steam as the gasifying agent with the same pressure and vary the flow rate. The temperature of the gasifier is controlled between 750°C and 950°C, while the agent flow rate is regulated according to the S/B ratio, which ranges from 0.2 to 1. Eq. (1) through (8) illustrate the gasification processes set in the gasifier reactor block. H_2, CO, CO_2, N_2, H_2O, and CH_4 are all present in the gasifier reactor's output stream, G-OUT.

In addition, the stream HYSUL is heated to the gasifier reactor temperature using a heater, characterized by the Heater block, while making the output stream from the heater block HYSUL1. In the mixer block, MIXER, HYSUL1, and the G-OUT are blended to form GAS1. Then, the output stream from the mixer approaches the cooler to cool down the GAS1, which is named producer gas. After passing through the cooler at 25°C with 1 bar pressure, the output stream is GAS2. That consist of H_2, CO, CO_2, N_2, H_2O, and CH_4. standing in for the gasifier's output. From the outlet stream of the cooler, the stream is sent to the Separator3, named the water separator, which will separate the water from the GAS2 and get the stream as syngas, named PRODUCT. That will be the final product from the model containing H_2, N_2, CH_4, CO, CO_2, and H_2S. In addition, Table 3 contains all information on the blocks and reactor utilized in this developed model.

Table 3 Characterization of blocks utilized in modeling [9].

ID Name	Tools description	Characterization
Decom	RYield	Yield reactor
Separator	Sep	Separator
STOIC	RStoic	Stoichiometric reactor
Separator2	Sep	Separator
Gasifier	Gibbs	Equilibrium reactor
Heater	Heater	Heater
Mixer	Mixer	Stream Mixer
Cooler	Cooler	Cooler
Separator3	Sep	Separator

4. Results and discussion

4.1 Model validation

The currently developed simulation and experimental results reported by Fremaux et al. [8] were the two models chosen to be verified. At a reactor temperature of 900°C, Fig.2 shows a high connection between the experimental results and the expected hydrogen output. The considerate experimental model [8] found that the ideal gasification temperature was 900°C.

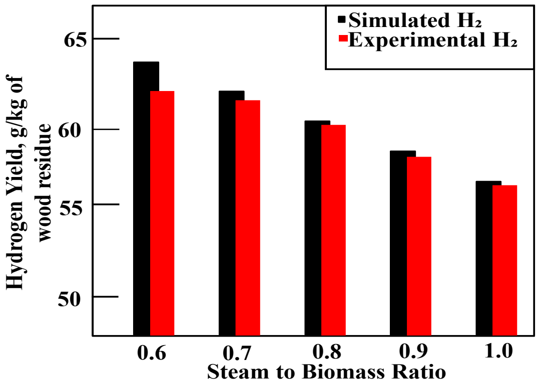

Fig.2 Hydrogen yield of wood residue Vs S/B ratio at a reactor temperature of 900°C

They described the increased hydrogen output in g/kg of wood waste to less tar formation at higher temperatures. The influence of various operational parameters, such as the temperature of the reactor and S/B ratio, on the composition of syngas and the H_2/CO ratio was evaluated using the validated model. The S/B ratio was modified between 0.6 to 1, while the temperature at the gasifier reactor varied between 750 and 950°C. All other circumstances were held constant while each variable was changed individually throughout the analysis.

4.2 Effect of gasification temperature

Fig.3 illustrates the impact of the temperature of the gasifier reactor at a constant rate of steam flow concerning the feed flow rate. The graph clearly shows that the concentration of CO and the concentration of H_2 rises with increasing the reactor temperature for both types of feedstocks. Also, it is shown that the concentration of CH_4 and CO_2 is decreased for both feedstocks. Here, it was observed that the characteristics of changing with varying reactor temperatures are the same for both biomass feeds. Also observed, the plot goes flat after 850°C reactor temperature at a constant flow of steam. Additionally, it was noted that the H_2 content stays nearly constant under all working circumstances, exhibiting a similar pattern to that documented in earlier research [15].

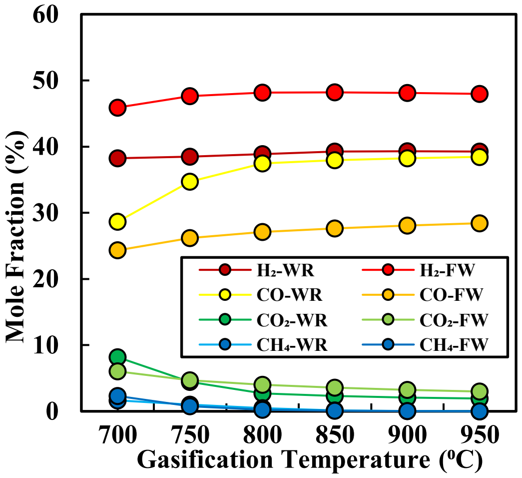

Fig.3 Mole Fraction Vs Gasification Temperature at 0.6 S/B Ratio

There is a fact for that type of varying characteristics, which is that the processes taking place inside the gasifier reactor were considered to have adequate dwell time and equilibrium reaction. The main focus of the investigation of syngas yield was reactor temperature and steam flow rate with respect to feed flow. According to the results, endothermic processes were encouraged by increased gasification temperatures, which decreased the concentrations of CH_4 and CO_2 while raising H_2 and CO outputs. Methane decrease mainly was described as the prevalence of methane reforming at high temperatures. In contrast, the Boudouard, water-gas, and steam methane reforming were the main reactions causing these trends.

Fig.4 illustrates how gasification temperature affects the syngas yield (Nm^3/kg) and lower heating value (LHV, MJ/kg) for WR and FW feedstocks. The analysis was conducted across a temperature range of 700°C to 950°C at a constant steam flow rate at the gasifier reactor. Syngas yield and LHV for both feedstocks gradually increase up to 850°C. The value of syngas yields 1.25 Nm^3/kg and 1.4 Nm^3/kg for WR and FW, respectively. The amount of LHV shown is around 11 MJ/kg and 12 MJ/kg for both WR and FW, respectively, beyond which the values stabilize through 950°C.

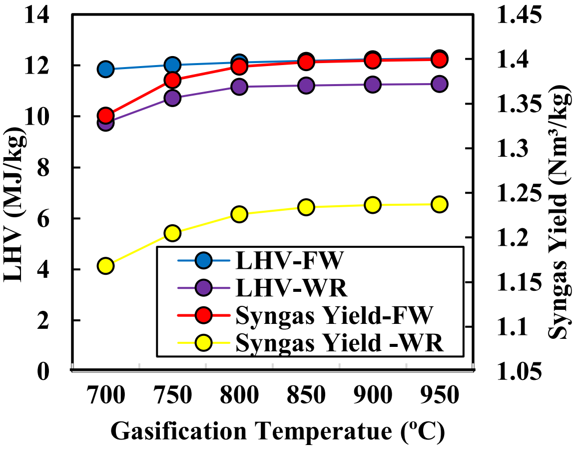

Fig.4 LHV & Syngas Yield Vs Gasification Temp at 0.6 S/B Ratio

Fig.5 illustrates how gasification temperature affects the H_2/CO fraction of the syngas content at an S/B ratio of 0.6. The H_2/CO ratio decreases as reactor temperature rises, which is attributed to increased CO in syngas while H_2 concentration remains nearly constant. It is suggested that the Boudouard reaction outweighs the water-gas reaction across the range of temperatures.

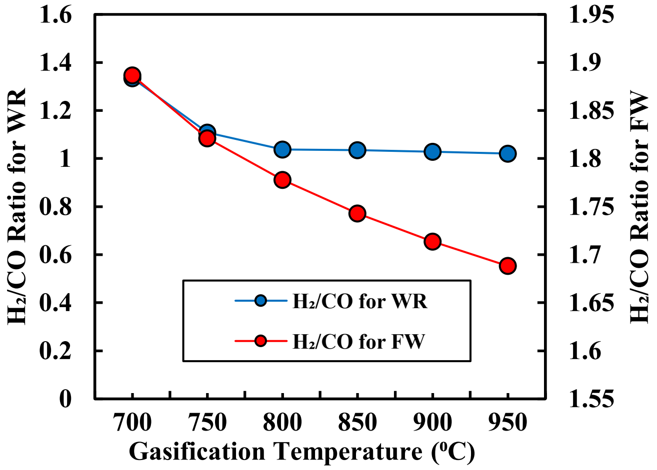

Fig.5 H_2/CO molar ratio Vs Gasification Temp at 0.6 S/B Ratio

At the same time, while the water-gas reaction also generates H_2, the S/B ratio of 0.6 limits the availability of steam, constraining the extent to which this reaction can produce additional H_2. Consequently, the H_2 concentration remains relatively constant. This temperature-induced increase in CO production, with minimal impact on H_2 concentration, leads to a decrease in the H_2/CO molar ratio as the reaction temperature rises.

4.3 Impact of steam to biomass (S/B) ratio

In the gasifier with reactor temperature at 700°C for WR and FW feedstocks, Fig.6 depicts the impact of the (S/B) ratio, which ranges from 0.5 to 1, on the composition of the syngas. It was found that while the levels of CO reduced, the concentration of CO_2 increased somewhat as the S/B ratio increased. Up to a S/B ratio of 0.8, the H_2 concentration gradually decreased; beyond that, it stayed steady.

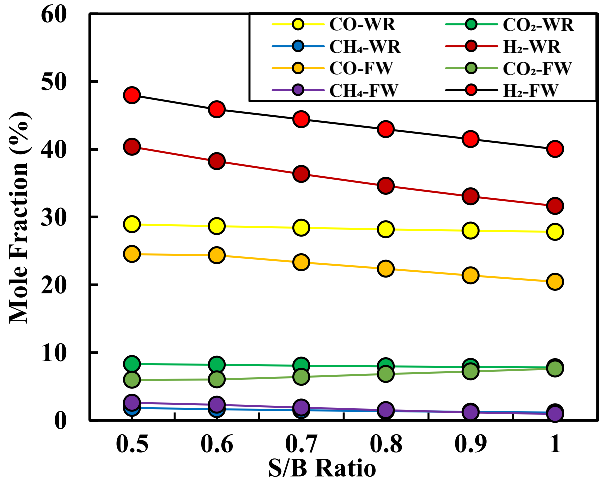

Fig.6 Mole Fraction Vs S/B Ratio at Gasification Temp (700°C)

Higher steam input causes changes in reaction equilibria, which accounts for these data. A modest increase in CO_2 and a decrease in CO levels result from the water-gas shift reaction. Fig.7 illustrates the impact of the S/B ratio, ranging from 0.5 to 1, on syngas yield (Nm^3/kg) and LHV (MJ/kg), evaluated at a temperature of 700°C for both feedstocks. Results indicate that syngas yield and LHV decrease as the S/B ratio approaches 0.8, after which they level off with minimal further change.

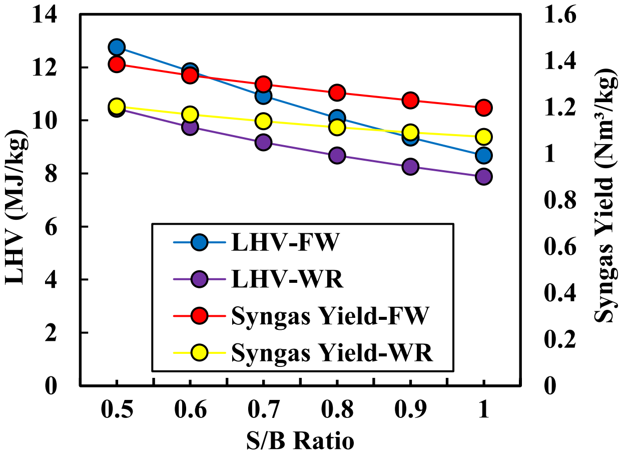

Fig.7 LHV & Syngas Yield Vs S/B Ratio at Gasification Temp (700°C)

This pattern arises because increased steam input enhances the water-gas shift reaction, converting more CO into CO_2 and H_2, reducing the CO concentration in the syngas. The reduction in CO concentration contributes to a decline in syngas yield and LHV up to an S/B ratio of 0.8.

Fig.8 illustrates that for the wood residue, the H_2/CO ratio decreases as the S/B ratio enhance, while for food waste, the H_2/CO ratio exhibits an upward trend with increasing S/B ratio. Because of the distinct composition and reactivity of each type of biomass feedstock. A higher S/B ratio in wood residue promotes a gentle water-gas shift reaction, converting the molar ratio of H_2/CO.

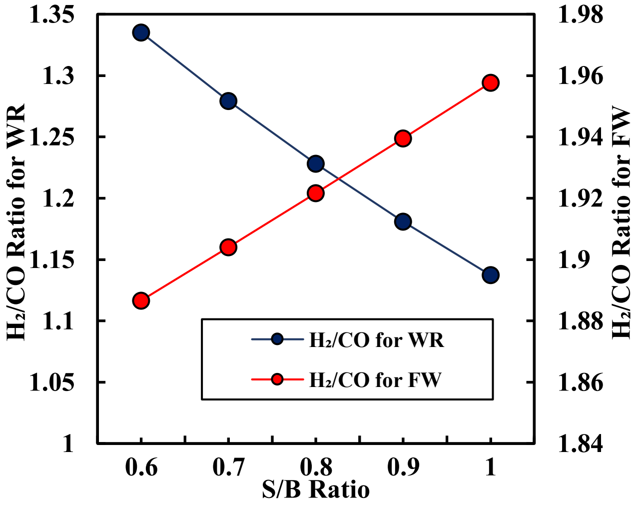

Fig.8 H_2/CO molar ratio Vs S/B Ratio at Gasification Temp (700°C)

In addition, food wastes have higher moisture content, which is the reason for enhanced hydrogen production in the same steam flow rate with respect to biomass at the gasifier reactor through steam reforming, thereby raising the H_2/CO ratio.

5. Conclusion

This study examined the effects of gasification temperature and steam-to-biomass (S/B) ratio on syngas yield, lower heating value, and product gas composition for wood residue and food waste feedstocks. However, the results indicate that increasing gasification temperature enhances syngas yield and LHV up to around 850°C. The yield values are around 1.4 Nm^3/kg and LHV around 12 MJ/kg at this temperature, after which the values stabilize due to reaction equilibrium. Additionally, rising S/B ratios reduce syngas yield and LHV, up to 0.8, due to increased CO_2 formation via the water-gas shift reaction. Regarding product composition, the H_2/CO molar ratio decreases with increasing S/B ratio for wood residue but increases for food waste, highlighting feedstock-specific reactions. These findings underscore the need to optimize gasification parameters according to feedstock characteristics to maximize energy efficiency and enhance syngas quality.

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NOMENCLATURE

S/B : steam to biomass ratio
p : pressure, bar
T : température, ºC