

Performance Investigation of Biomass Gasification for Syngas and Hydrogen Production Using Aspen Plus

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Abstract

This study presents a reliable model using Aspen Plus process simulator capable of performing a sensitivity analysis of the downdraft gasification linked to hydrogen production unit. Effects of key factors, including gasification temperature and steam to biomass ratio (SBR) on the syngas composition, calorific value of syngas and hydrogen production are discussed and then the optimal conditions for maximum hydrogen production are extracted. The model is validated by experimental and other modeling data and found to be in great agreement. The sensitivity analysis results obtained by only using air as gasification agent indicate that higher temperatures are favorable for a product gas with higher hydrogen content and calorific value. Moreover, steam consumption as gasifying agent leads to increasing the hydrogen content and heating value of the syngas compared to the use of air as gasification agent. Finally, the results show that the optimal conditions to have the highest value of hydrogen output from sawdust downdraft gasification are 800°C as gasifier temperature and 0.6 for SBR.

Keywords

Biomass Gasification, Syngas, Hydrogen, Simulation, Parametric Analysis

1. Introduction

Today, the widest contribution to world's energy supply is related to fossil fuels and it could reach more than 80% among different energy suppliers by 2040 if continued in the same way [1]. This structure will lead to catastrophic conse-

quences in view of environmental damage due to greenhouse gas emissions (GHGs) connected with fossil fuels [2] [3] [4]. This situation encourages in replacement of fossil fuels with renewable energy sources and among these energy alternatives, biomass as a carbon-neutral fuel is considered as one of the most promising sources that have the potential to replace fossil fuels as well it mitigates the usual problems in other renewable energy sources, like the intermittent nature of wind and solar energy [5] [6] [7]. Moreover, biomass feedstocks are not only utilized as substitution, but also highly beneficial for hydrogen production [8]-[16].

The most important biomass feedstocks which have high potential sources of energy include forest residues from industries like wood chips, sawdust, and bark and agricultural residues like straw, husk and bagasse [17] [18] [19]. There are three main thermochemical conversion processes like direct combustion, gasification and pyrolysis that can transform biomass to gas. Direct combustion produces heat while the two latter can produce various types of energy carriers that can be converted into fuels. However, over the past decades, biomass gasification has been regarded as a very promising technology, because of the large potential and the option of advanced applications [13] [20]-[25]. Gasification is the partial oxidation of biomass at high temperatures in the presence of a gasification agent, which can be steam, oxygen, air or a combination of these. The resulting gas mixture is called syngas or producer gas and can be used in various processes to produce liquid fuels such as methanol, ethanol and Fischer-Tropsch diesel, and gaseous fuels, such as hydrogen and methane.

Modeling and simulation could be very helpful tools at exploitation of the biomass gasification potential, while the fuel and the considered method are intricate and various factors affect the output of the system [26] [27] [28] [29] [30]. Mathematical models are much more beneficial in comparison to experimental works because of easy investigation of different scenarios at less time and costly procedures. They are also so important and critical technique for understanding and predicting the system behavior and assessment of impacts of various parameters on the system performance [31] [32] [33]. They have also the advantage of preventing and allowing us to study different scenarios escaping to time-consuming and costly procedures [34] [35]. To avoid the elaborations through the gasification plant and establish a simple and practical model for investigation of the gasification reactions, reactors and other required processes the Aspen Plus simulator is employed [36] [37]. Aspen Plus is a serial modular and equation-oriented simulation program relying on the mass and energy balances relations and phase equilibrium data, which has been employed for simulation of various systems containing the conventional coal and biomass gasification process and also plasma gasification process [28] [38] [39] [40] [41] [42].

Han *et al.* [28] established a simulation model for the downdraft biomass gasification by using Aspen Plus by minimizing Gibbs free energy modified with restricted chemical reaction equilibrium in the reduction zone. The model was confirmed by the experimental data of downdraft hardwood chips gasification.

Moreover, sensitivity analysis was carried out to investigate the effects of gasification temperature, equivalence ratio, and biomass moisture content on the syngas compositions. The developed model showed that all the studied parameters had a key impact on the syngas components. Kaushal and Tyagi [41] created a mathematical model of bubbling fluidized biomass gasification in ASPEN PLUS by considering tar generation and cracking. Results proved that consideration of tar and its kinetics notably modifies the model performance. Doherty and Reynolds [43] developed a model in Aspen Plus for a fast internally circulating fluidized bed (FICFB) gasifier. Begum *et al.* [44] also developed an Aspen Plus model for an integrated fixed bed gasifier and predicted the steady-state performance of the model for different biomass feedstocks. Sreejith *et al.* [45] created an equilibrium model that relied on Gibbs free energy minimization for steam gasification of biomass using the Aspen Plus process simulator. They assumed that carbon is fully converted to product gases and no tar content is present in the gaseous product.

From the above-mentioned studies, it can be concluded that the simulation modeling of biomass gasification by applying the Aspen Plus simulator is varied. The recent tendency is towards addition of sub-models for consideration of some specific aspect of the gasification process, like tars to modify its prediction ability. Therefore, the aim of this research is development of a reliable simulation model by applying the Aspen Plus simulator capable of performing a sensitivity analysis of the sawdust downdraft gasification for syngas and hydrogen production.

2. System Description and Process Simulation

2.1. System Description

A model for sawdust downdraft gasification was established in the Aspen Plus simulator. The developed model can control unconventional materials like biomass and ash, which are included in various processes through the gasification plant. The model includes several operational units like reactors, separators, compressor, heat exchangers and various streams. The system considered in this work is shown in **Figure 1**. Sawdust was used as the biomass feedstock. The characteristics of sawdust are shown in **Table 1** [46]. Through the drying step moisture content of the biomass is decreased to less than 5%. Then the dried biomass in the pyrolysis step is decomposed to the volatile materials and char. The pyrolysis output goes then to the gasification step and there models the partial oxidation and gasification reactions by minimizing Gibbs free energy, which formulation can be found in literature [46] [47]. The applied modeling approach in this work is non-stoichiometric which means that firstly all the species to be included in the simulation are selected (in principle, all the chemical species that the modeler might be in the gasifier effluent in non-negligible amounts) and then the resulting minimum Gibbs energy distribution among these chemical species for a given feed composition is computed (which can be specified simply

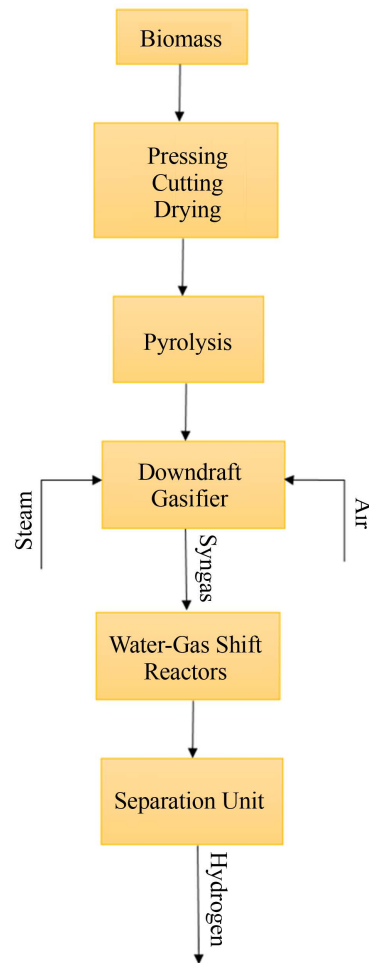


Figure 1. Process flow diagram for gasification integrated with hydrogen production.

Table 1. Ultimate and proximate analysis of feedstock.

	Sawdust
Proximate analysis	
Proximate analysis (wt%)	
Moisture	7
Volatile matter (VM)	81.72
Fixed carbon (FC)	17.2
Ash	1.08
Ultimate analysis	
Elemental analysis (wt%-dry basis)	
Carbon	46.46
Hydrogen	5.82
Nitrogen	0.19
Oxygen	46.45

as the elemental composition of the feed. Indeed, grammatically the only input needed to specify the biomass is its elemental composition and proximate analysis data [48] [49]. Therefore, non-stoichiometric models could be particularly proper for cases in which all the possible reactions occurring in the system are not fully known as is the case of gasification.

2.2. Simulation Modeling by Aspen Plus

Figure 2 shows the Aspen Plus flow chart of the process modeling for sawdust gasification with agent of air/steam. The developed model in this work contains two main parts of gasification and linked to the hydrogen production unit.

The gasification process starts with the biomass feedstock (BIOMASS stream) as the non-conventional input to the system. In this simulation, HCOALGEN and DCOALIGT were employed for calculation of enthalpy and density of biomasses and ash based on the proximate analysis, ultimate analysis, and sulfur analysis of the feedstocks and ash. Peng-Robinson equation with Boston-Mathias alpha function (PR-BM) was applied to estimate all physical properties of the conventional components in gasification process [50] [51] [52].

Drying is the first step of the gasification process which was simulated in the DRIER block. The purpose of this step is to decrease the moisture content of the biomass to less than 5%. The Aspen Plus stoichiometric reactor (RSTOIC) was employed for simulation of the moisture evaporation [18] [53]. A Fortran subroutine water calculator was also modeled to handle the drying process. The moisture content in biomass is partially evaporated and then separated by using a separator model (SEP1) through split fractionation of the components and the evaporated moisture is drained out from the system [54]. At the next part, the dehydrated feedstock is moved into the pyrolysis. RYIELD, the yield reactor, was employed for modeling of the biomass pyrolysis in Aspen Plus (shown in **Figure 2** with “PYROL”). In this step, biomass is transformed to its constituting components C, H, O, N and ash, by specifying the yield distribution based on the biomass ultimate and proximate analysis. The yield distribution is a required procedure of RGIBBS chemical equilibrium by minimizing Gibbs free energy

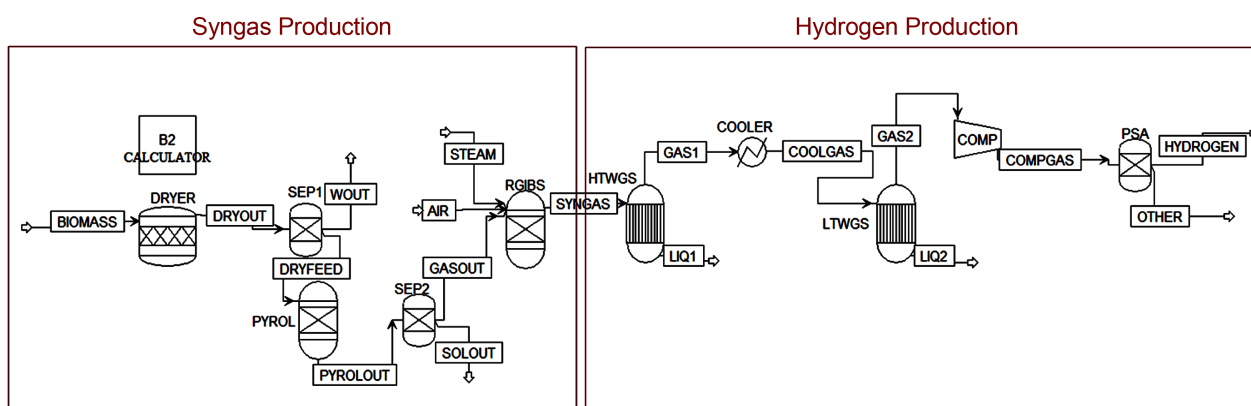


Figure 2. Aspen Plus flow chart of gasification integrated with hydrogen production.

due to the inability of the Gibbs reactor to deal with non-conventional components such as biomass [55]. In this step, the feedstock is converted to volatile materials (VM) and char. Tars are neglected in this phase since downdraft gasification is recognized to produce insignificant tar contents [41] [56]. It is assumed that the total yield of volatiles is equal to the volatile content of the biomass and the total yield of chars is equal to fixed carbon and ash contents determined by proximate analysis. The yield distribution of biomass into its components has been specified by Fortran subroutine in yield calculator.

The last phase of gasification is carried out in a RGIBBS reactor that is based on the Gibbs free energy minimization as a model for multiphase chemical equilibrium. This reactor calculates the output composition by minimizing the Gibbs free energy, and reaching a complete chemical equilibrium. In this block, air or mix of air/steam is introduced as a gasification agent through the system [12] [57].

Then the product syngas goes to the water-gas shift process. For this stage, two water-gas shift reactors were applied since water-gas shift reaction is moderately exothermic, and it tends to shift to the left side at high temperature. One is at higher temperature (HTWGS) and the other is at lower temperature (LTWGS). In the HTWGS reactor, there is a first low conversion of CO with quick kinetics (based on Equation (1)), but it is not possible to go beyond the equilibrium curve, thus the LTWGS reactor was used [58].



In the LTWGS reactor, by reducing the operation temperature, it was possible to obtain higher conversion. HTWGS and LTWGS have been simulated at 400°C and 200°C with two Requill reactors, respectively [25]. Requill is equilibrium reactor for which the chemical and phase equilibrium are determined by stoichiometric calculations. Then to reach a high purity of hydrogen, a PSA unit was employed [59] [60]. A separation efficiency of 70% for hydrogen and an input pressure of 7 bars for simulation of PSA were considered from the optimal values found in the literature [10] [61] [62] [63]. Pressurization was achieved with a compressor, COMP before the PSA and the PSA outlet stream, denoted as HYDROGEN.

3. Model Validation

To validate the Aspen Plus model established in this paper, the developed simulation model was performed based on conditions presented in Jayah *et al.* [64]. Rubber wood was considered as feedstock and its proximate and ultimate analyses were brought in Table 2. The comparison of Aspen Plus results in this paper with the experimental results extracted from Jayah *et al.* [64] for rubber wood downdraft gasifier agented by air and also with the results obtained from the developed model by Tavares *et al.* [55] were shown in Figure 3. The operational factors were fixed on temperature of 1100 K, 16% mole of moisture per mole of rubber wood and 464.7 mol of air per mole of feedstock.

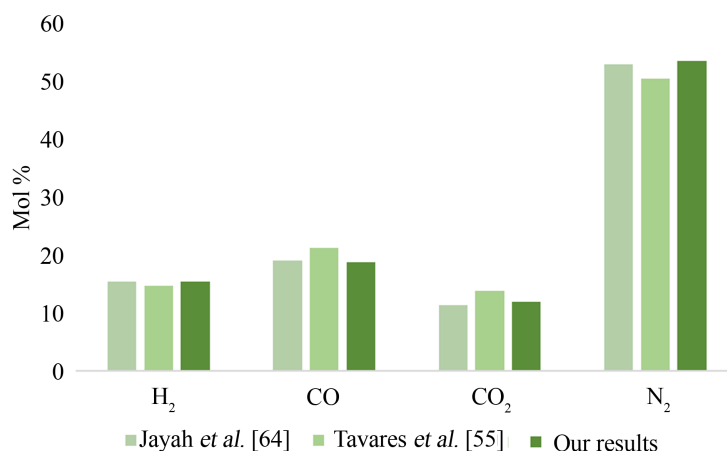


Figure 3. Comparison of mole fractions of syngas composition among our work and experimental and modeling results in literature.

Table 2. Ultimate and proximate analysis of rubber wood.

Rubber wood	
Proximate analysis	
Proximate analysis (wt%)	
Volatile matter (VM)	80.1
Fixed carbon (FC)	19.2
Ash	0.7
Ultimate analysis	
Elemental analysis (wt%-dry basis)	
Carbon	50.6
Hydrogen	6.5
Nitrogen	0.2
Oxygen	42

The comparison proves that the Aspen Plus results gained in this research are all in great agreement with the experimental results. In addition, the Aspen Plus results extracted in this paper show much better prediction of the syngas composition compared to the developed model by Tavares *et al.* [55]. The deviation of the Aspen Plus results from literature values (compared data) has been calculated by the relative error [65]:

$$\text{Relative error (\%)} = 100 \times \frac{\text{Model value} - \text{Experimental value}}{\text{Experimental value}} \quad (2)$$

Table 3 shows the relative errors between experimental values with Aspen Plus results in this work as well as with the model results obtained in Tavares *et al.* [55]. It can be seen that the error calculated from the developed model in this paper is less than 5% for all components.

Table 3. Relative error calculated based on Equation (2).

	Error of our results in comparison to experiment	Error of Tavares <i>et al.</i> [55] in comparison to experiment
H ₂	-0.65	-4.52
CO	-1.57	10.99
CO ₂	5.26	21.93
N ₂	1.13	-4.54

4. Results and Discussion

The established model has been employed to evaluate the effect of various parameters such as gasifier temperature, steam-to-biomass ratio (SBR) and steam injection on syngas composition, lower heating value (LHV) and hydrogen production for sawdust with the proximate and ultimate analysis listed in **Table 1**.

4.1. Impact of Temperature on Syngas Composition

Gasifier temperature influences significantly on the output products of the system. It can be explained by that several chemical reactions occurring inside the gasifier are endothermic. Hence, higher temperatures favors for endothermic reactions products. Impact of gasification temperature on syngas composition was studied in the window of 500°C - 1500°C. While the mass flow rate of air to fuel ratio was set to 1.8, moisture content reduced to 5%, and biomass feeding rate was 1000 kg/hr. **Figure 4** presents the molar fraction of syngas compositions a function of the gasification temperature. Obviously, by increasing of the gasification temperature the formation of a product gas with higher hydrogen and carbon monoxide contents is promoted. The increase in CO and H₂ concentration is because of the combined effect of boudouard, steam methane reforming and water-gas reaction. These reactions are endothermic in nature and thus are preferred at higher temperatures. However, methane and carbon dioxide contents show an opposite trend because of exothermic nature of water gas shift and methanation reaction that make them unfavorable by increasing temperatures.

4.2. Impact of Temperature on Syngas LHV

Lower heating value (LHV) of fuel is described as the amount of heat released by fully combusting a specified value of fuel deducted by the vaporization heat of water in the combustion product. LHV can be calculated as [66] [67]:

$$\text{LHV}_{\text{syngas}} \left(\text{kJ/N} \cdot \text{m}^3 \right) = 4.2 \times \left(30 \times y_{\text{CO}} + 25.7 \times y_{\text{H}_2} + 85.4 \times y_{\text{CH}_4} \right) \quad (3)$$

where y presents molar fractions of components in the gas product (dry basis) that are extracted from the simulation results. **Figure 5** shows the impact of the temperature on the produced syngas LHV. Firstly, LHV increased abruptly from 2.75 MJ/Nm³ at 500°C to 5.03 MJ/Nm³ at 800°C and then almost became

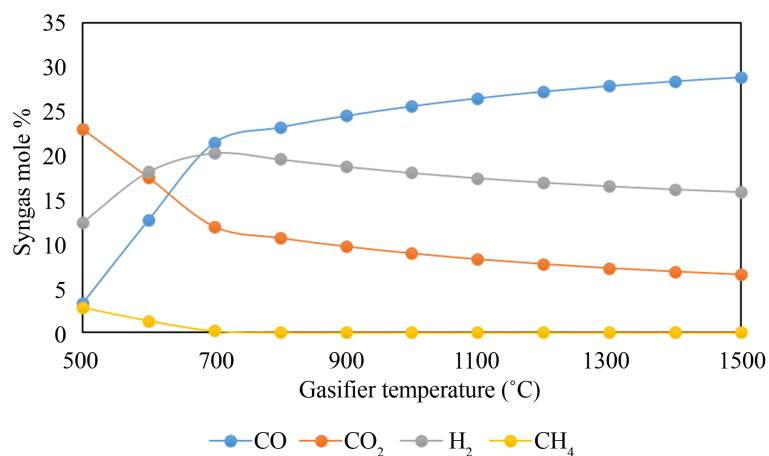


Figure 4. Impact of gasification temperature on molar fraction of syngas compositions (at dry basis).

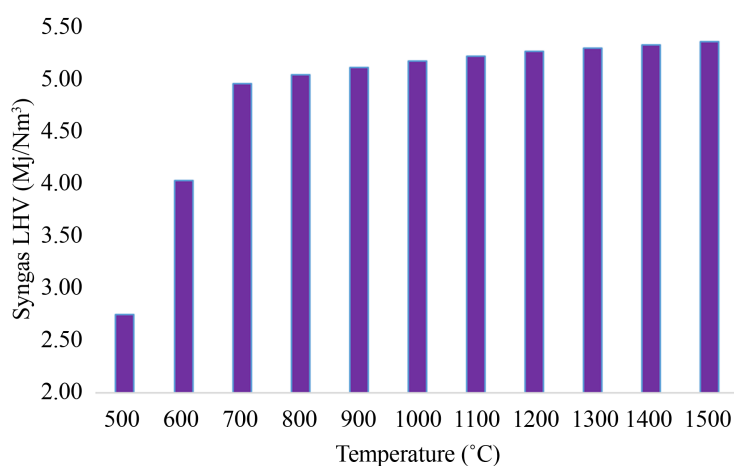


Figure 5. Impact of gasification temperature on molar fraction of syngas LHV.

constant. LHV increases till 800°C due to the increase in H₂, CO, and CH₄ concentrations. After 800°C, LHV do not change much since reduction of H₂ content and slightly extension of CO content.

4.3. Impact of Steam to Biomass Ratio (SBR) on Syngas Composition

The steam to biomass ratio (SBR) is specified as the mass flow rate of the steam injected to the gasification reactor divided by the biomass mass flow rate in dry basis, and is one of the most key factors affecting on the steam gasification [12]. The most important benefit of utilizing steam as gasifying agent is the increment of the molar fraction of hydrogen. Increasing of steam injection to the system will extend the water concentration, leading to more water shift reactions. The SBR has been changed in the window of 0.1 to 0.9 by holding the other variables constant. **Figure 6** depicts the syngas molar fractions as a function of SBR.

As seen in **Figure 6**, steam consumption as a gasifying agent grows the partial pressure of water inside the gasifier which is beneficial for the water gas shift and

steam reforming reactions, leads to increase in H_2 and CO_2 and the decrease in CO production.

4.4. Impact of SBR on Syngas LHV

The impact of steam to biomass ratio on the LHV of syngas at fixed AFR of 1.8 was depicted in **Figure 7**. It could be seen that LHV of syngas reduces from 4.99 Mj/Nm^3 at $SBR = 0.1$ to 4.5 Mj/Nm^3 at $SBR = 0.9$. In fact, by growth in steam feeding to the system, production of carbon monoxide in the syngas is degraded because of the water gas shift reaction, so the syngas LHV moves down. Additionally, owing to water gas shift reaction, hydrogen value in the syngas is added but its degree of increase is not enough that be able to overcome the effect of CO reduction.

4.5. Impact of Temperature and SBR on Hydrogen Production

Combination of two significant factors of gasification temperature and SBR, make it possible to optimize the operational conditions to have maximum amount of hydrogen production. This investigation was presented in **Figure 8**. It

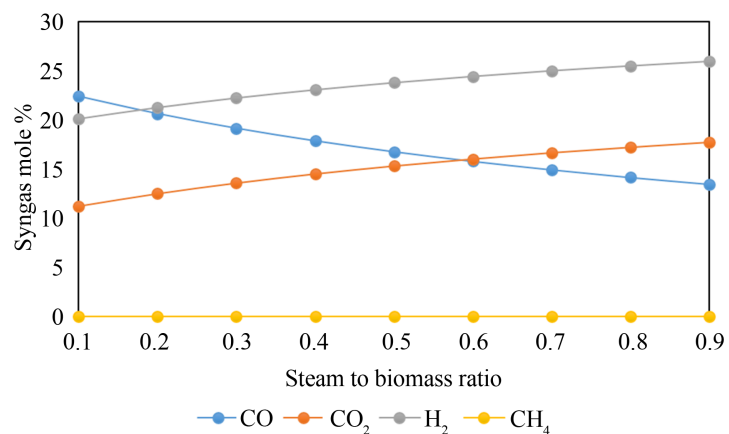


Figure 6. Impact of SBR on molar fraction of syngas compositions.

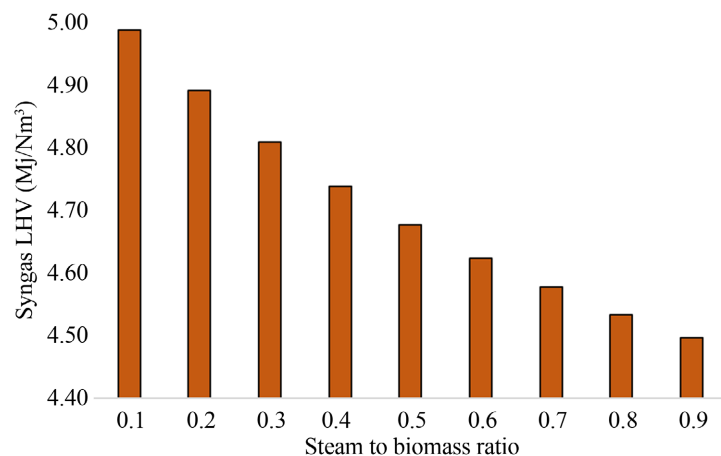


Figure 7. Impact of SBR on syngas LHV.

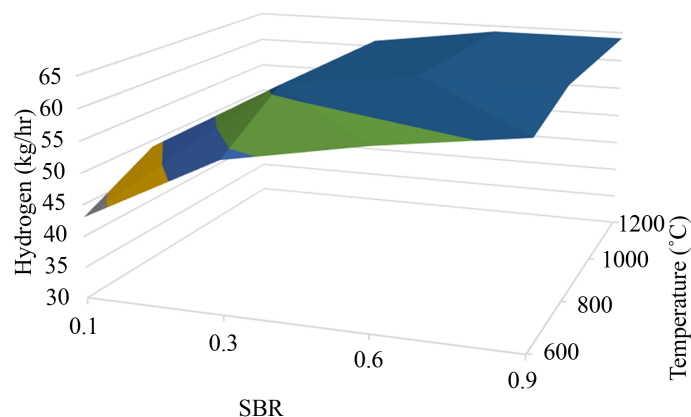


Figure 8. Impact of temperature and SBR on hydrogen production.

could be observed that higher SBR leads to higher hydrogen production, moreover the mass flow rate of hydrogen at different SBR makes better by growing the temperature. While this increasing trend is saturated till the specific operational conditions that are considered as optimal conditions, the optimal condition to have highest value of hydrogen production from sawdust downdraft gasification are 800 °C as gasifier temperature and 0.6 for SBR.

5. Conclusion

In this paper, a detailed downdraft biomass gasification link to hydrogen production unit was modeled by applying Aspen Plus simulator. Sawdust as lignocellulosic biomass was considered as the input feedstock to the system. Parametric analysis was carried out by varying gasifying agent composition, gasification temperature from 500 °C to 1500 °C and mass flow rate of stem to biomass ratio from 0.1 to 0.9.

- The developed simulation model was validated with the experimental study conducted by Jayah *et al.* and modeling study performed by Tavares *et al.* on rubber wood downdraft gasification. The comparison proved that the simulation results showed that the Aspen Plus results gained in this research are all in great agreement with the experimental results, with error of less than 5%. In addition, the Aspen Plus results extracted in this paper show much better prediction of the syngas composition compared to the developed model by Tavares *et al.*
- Hydrogen concentration in the syngas is increased by extending the gasifier temperature but it is saturated at 700 °C that is around 20%. While, by increasing SBR from 0.1 to 0.9, molar fraction of hydrogen increases from 20% to 26%.
- The temperature and SBR present opposite effect on the syngas LHV. It is because of the CO content. Molar fraction of CO increases with temperature and reduces with SBR and CO has a higher influence than H₂ in the LHV.
- Higher SBR leads to higher hydrogen production, moreover, the mass flow rate of hydrogen at different SBR makes better by growing the temperature.

While this increasing trend is saturated till the specific operational conditions, the optimal conditions to have the highest value of hydrogen output from sawdust downdraft gasification are 800°C as gasifier temperature and 0.6 for SBR.

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Authors' Contributions

Sahar Safarian: Conceptualization, Methodology, Simulation, Validation, Formal analysis, Investigation, Resources, Writing of original draft, review & editing. Runar Unnthorsson: Supervision, Funding. Christiaan Richter: Software & Supervision.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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