



 **Opin vísindi**

This is not the published version of the article / Þetta er ekki útgefna útgáfa greinarinnar

Author(s)/Höf.: Sahar Safarian, Rúnar Unnpórsson, Christiaan Richter
Title/Titill: Hydrogen production via biomass gasification: simulation and performance analysis under different gasifying agents
Year/Útgáfuár: 2021
Version/Útgáfa: Pre-print (óritrýnt handrit)

Please cite the original version:

Vinsamlega vísið til útgefnu greinarinnar:

Safarian, S., Unnthorsson, R., & Richter, C. (2021). Hydrogen production via biomass gasification: simulation and performance analysis under different gasifying agents. *Biofuels*, 1-10.
doi:<https://doi.org/10.1080/17597269.2021.1894781>

Rights/Réttur: Copyright © 2021 Informa UK Limited

Hydrogen production via biomass gasification: Simulation and performance analysis under different gasifying agents

Sahar Safarian^{*}, Runar Unnthorsson, Christiaan Richter

Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, University of Iceland, Hjarðarhagi 6,
107 Reykjavík, Iceland

Email: *sas79@hi.is (S. Safarian)

Abstract

This study develops a new simulation model by ASPEN Plus for gasification integrated with water-gas shift reactors and product recovery unit for hydrogen production. Timber and wood waste (T&WW) as a lignocellulosic biomass was also considered as the input feedstock to the system. Then, the model is applied to investigate the effect of two agents of air and a mixture of air-steam under different operating conditions of temperature and steam to biomass ratio (SBR). The results reveal that the produced hydrogen through the air-steam gasification is at the highest points for all studied temperatures and it would be maximum (44.37 Kmol/hr per 1 ton T&WWs) at 700 °C. The hydrogen production efficiency (HPE) can be also raised, stemming from the growth of H₂. It values 39.2% at SBR = 0.1 that grows to 70% at SBR = 0.9. The optimum SBR lies between 0.7-0.8 that specific mass flow rate of hydrogen would be higher than 0.1 kg_{hydrogen}/kg_{T&WW}.

Keywords: Hydrogen production, Biomass gasification, Water-gas shift reactor, Process simulation, Gasifying agents.

Introduction

Growing concerns about the depletion of fossil fuels, energy security and environmental impacts due to burning of the fossil fuels have encouraged the decision makers in the energy sector to substitute fossil fuels with renewable and sustainable energy alternatives [1-5]. Among the renewable energies, biomass and hydrogen have received significant attention as they can increase the global energy sustainability and reduce greenhouse gas emissions [6-10]. Globally, biomass has the third widest energy source after coal and oil [11] and it includes plenty advantages such as it is inexhaustible, it can be easily stored, and its CO₂ emissions is considered climate-neutral, since the CO₂ released through the biofuel combustion is almost equal to the CO₂ value absorbed by biomass during its lifetime [12,13].

There are various technologies for conversion of biomass to product gas, including thermochemical, biochemical and mechanical extraction methods. Thermochemical conversion methods can be classified into: combustion, gasification, pyrolysis and liquefaction [14,15]. Among these methods, biomass gasification is a promising technology to convert different feedstocks for various energy purposes [16-18]. This complex thermochemical process converts the lignocellulosic materials into a more valuable gas known as syngas by a series reactions at high temperatures [19-21]. The gasification process takes place in the presence of gasification agents such as air, steam, oxygen, or a mixture of them. Air gasification produces syngas with LHV in the range of 4-7 MJ/Nm³ and if steam is used instead of air the syngas produced has a LHV in the range of 10-15 MJ/Nm³ and the hydrogen yield is higher, as a result of water gas shift reaction [22,23]. However, it would be more beneficial to consider a mixture of air and steam as the oxidizing agent because biomass steam gasification requires external heat due to the endothermic steam reforming reactions involved [24].

The gasification process consists different steps of drying of the wet feedstocks, pyrolysis of the dried feedstocks and the reaction part containing oxidation, reduction and cracking [15,25]. Syngas as a result of biomass gasification, contains mainly carbon monoxide,

hydrogen, carbon dioxide, methane and traces of higher hydrocarbons, can be used for polygeneration purposes such as thermal heat, power generation or to produce hydrogen fuel [26-28]. Hydrogen has the highest energy density among all hydrocarbons fuels which is about 122 kJ/kg [29] and it can be used as a clean energy source for fuel cells, clean energy carrier for heat supply, and transportation purposes [30-32]. Several technologies were developed to produce hydrogen, like conventional methane steam reforming, biological processes, biomass gasification, biomass pyrolysis, electrolysis, and thermochemical water splitting [19,33].

Biomass gasification as an attractive technology for conversion of various types of biowastes to energy, has been known as a clean and efficient way of producing hydrogen [34,35]. Biomass gasification is of significant interests due to the facts that (a) the process is fast, (b) the process is efficient, (c) biomass is environmentally friendly, (d) biomass is renewable, etc. [36,37]. Performance analysis of biomass gasification systems has been studied in many researches [4,27,38-46]. However, there are just a few studies on performance analysis of integrated gasification-hydrogen production [10,28,47].

Meramo-Hurtado et al., [48] addressed the modeling and evaluation of a biomass gasification topology for hydrogen production, employing process simulation along with an environmental and inherent safety analysis. The presented pathway considered for cassava and rice waste as renewable raw materials based on their vast availability in north Colombia regions. they employed Aspen Plus process simulation software to model the process, setting biomasses and ash content as nonconventional solids in the software and inclusion of FORTRAN subroutines for handling solid properties. However, their focus is mainly on environmental evaluation applying based on the waste reduction algorithm (WAR) and safety assessment that involve a comprehensive approach based on the inherent safety index (ISI) and the process route index (PRI) methods. Marcantonio et al., [28] studied the gasification of hazelnut shells within a circulating bubbling fluidized bed gasifier through a quasi-equilibrium approach developed in the Aspen Plus environment and used to validate and improve an existing bubbling fluidized bed gasifier model. The gasification unit was integrated with a water-gas shift (WGS) reactor to increase the hydrogen content in the outlet stream and with a pressure swing adsorption (PSA) unit for hydrogen separation. The amount of dry H₂ obtained out of the gasifier was 31.3 mol%, and this value increased to 47.5 mol% after the WGS reaction. Shayan et al., [10] investigated the hydrogen production from biomass gasification using various agents and compared theoretically, from the viewpoints of the first and second thermodynamics laws. Gasification of wood and paper, were assessed using four gasification agents of air, oxygen-enriched air, oxygen and steam. A parametric study was also conducted to assess the effects of key operating parameters on the hydrogen concentration and calorific value of product gas, energy and exergy efficiencies of the process and exergy destruction rate at different operating conditions. The results indicate that the higher values of hydrogen production is associated respectively with using steam, oxygen, oxygen-enriched air and air as the gasification agents. Also, it is concluded that for the gasification process the highest value of sensible energy efficiency is obtained for air gasification, while the highest exergy efficiency, as a rational criterion, is obtained for steam gasification for which the calorific value of the producer gas can reach to higher than 11 MJ/Nm³. Nakyai et al., [49] studied, the effects of various types of gasifying agent, i.e., air and steam for the biomass

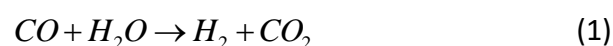
gasification with/without methane co-feeding through an exergoeconomic analysis. It is observed that the methane co-feeding can improve the energy and exergy efficiency. In exergoeconomic analysis, the specific exergy cost method was applied to investigate the unit cost of hydrogen. The economic reveal that the biomass gasification using air-steam as an agent with methane co-feeding presented the lowest unit hydrogen cost of 2.69 \$/kg and the unit exergy cost of hydrogen is 0.068 \$/kWh. Although there have been several studies on hydrogen production by using biomass gasification, the authors are not aware of any reported works on effect evaluation and sensitivity analysis of different agents and critical operating parameters on gasification performance and hydrogen production. Therefore, the objective of the present study is development of a new simulation model by using ASPEN Plus for the integrated gasification with hydrogen production from timber and wood waste (T&WW) as the feedstock. Then, the model is used to investigate the effect of two agents of air and a mixture of air-steam on the system performance. Moreover, two sensitivity analyses are carried out to study the impacts of the gasifier temperature and the steam to biomass ratio (SBR) on the syngas composition, low heating value (LHV) of syngas, hydrogen production and its efficiency. Thus, this study could provide a framework for defining the gasification, and hydrogen production plants to support equipment specification, and will be the basis for a future comprehensive environmental and techno-economic assessments.

Material and methods

System description

The system considered in this work is shown in Fig. 1. Timber and wood wastes (T&WW) were used as the biomass feedstock. The characteristics of T&WWs are brought in Table 1. Typically, the moisture in the biomass ranges from 5–60% that during drying, it is reduced to below 5%. In the pyrolysis step, the biomass is heated from with limited oxygen or air and under these conditions the volatile components in the biomass are vaporized. The oxygen supplied to the gasifier reacts with the combustible substances, producing CO₂ and H₂O. Some of this CO₂ and H₂O subsequently are reduced to CO and H₂ upon contact with the char produced from pyrolysis [50]. Moreover, the hydrogen in the biomass can be oxidized, generating water. The reduction reactions occurring inside the gasifier are endothermic, and the energy required for these reactions is provided by the combustion of char and volatiles. Reduction of the biomass yields combustible gases such as hydrogen, carbon monoxide, and methane through a series of reactions; the main reactions in this category are as follows (Table 2) [51,52]:

After gasification, the produced syngas undergoes the water-gas (W-G) shift reaction:



Which occurs in two reactors of high temperature shift and low temperature shift [53]. The gas from the W-G shift contains mainly H₂, CO₂, residual steam, and traces of CH₄ and CO; then to produce pure hydrogen, these gases is fed into the PSA system to obtain pure hydrogen.

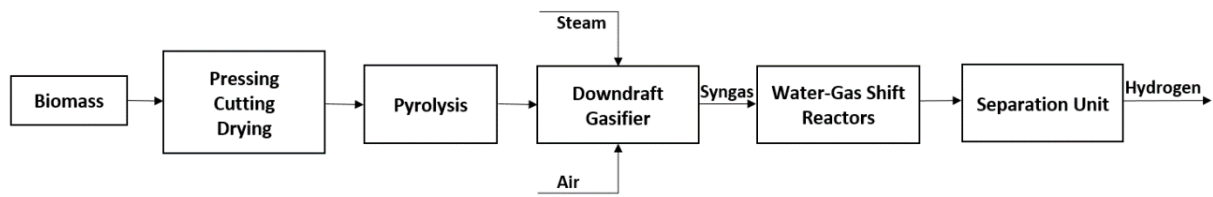


Fig.1: Structure of the biomass gasification-hydrogen production process.

Table 1. Ultimate and proximate analysis of feedstock [4,39]

Timber & wood waste	
Proximate analysis	
<i>Proximate analysis (wt%)</i>	
Moisture	5.01
Volatile matter (VM)	93.06
Fixed carbon (FC)	6.38
Ash	0.56
Ultimate analysis	
<i>Elemental analysis (wt%-dry basis)</i>	
C	56.8
H	7.28
N	0.18
Cl	0.82
S	0.07
O	34.29

Table 2: Main gasification reactions [51,52]

Heterogeneous reactions			
$C + O_2 \rightarrow CO_2 + 394 \text{ kJ/mol}$	Complete combustion		R1
$C + 0.5O_2 \rightarrow CO + 111 \text{ kJ/mol}$	Partial combustion		R2
$C + CO_2 \rightarrow 2CO - 172 \text{ kJ/mol}$	Boudouard		R3
$C + H_2O \rightarrow CO + H_2 - 131 \text{ kJ/mol}$	Water-gas		R4
$C + 2H_2 \rightarrow CH_4 + 75 \text{ kJ/mol}$	Methanation		R5
Homogeneous reactions			
$CO + 0.5O_2 \rightarrow CO_2 + 283 \text{ kJ/mol}$	CO partial combustion		R6
$H_2 + 0.5O_2 \rightarrow H_2O + 242 \text{ kJ/mol}$	H ₂ combustion		R7
$CO + H_2O \rightarrow CO_2 + H_2 + 41 \text{ kJ/mol}$	Water-gas shift (WGS)		R8
$CH_4 + H_2O \rightarrow CO + 3H_2 - 206 \text{ kJ/mol}$	Reforming		R9
H₂S and NH₃ formation reactions			
$H_2 + S \rightarrow H_2S$	H ₂ S formation		R10
$3H_2 + N_2 \rightarrow 2NH_3$	NH ₃ formation		R11

Simulation model

An equilibrium simulation model has been developed for biomass gasification integrated with W-G shift unit and separation unit for ethanol production by using ASPEN Plus version 10. Peng-Robinson equation of state with Boston-Mathias alpha function (PR-BM) was applied to calculate physical properties of the conventional components in the gasification process. HCOALGEN and DCOALIGT models were also employed for enthalpy and density of biomass and ash which are non-conventional components. MCINCPD stream comprising three substreams of MIXED, CIPSD and NCPD class, was also considered to define the biomass structure and ash streams which are not available in Aspen Plus component database [27,39,41,54,55]. The flow chart of the system simulated by using ASPEN Plus is shown in Fig. 2.

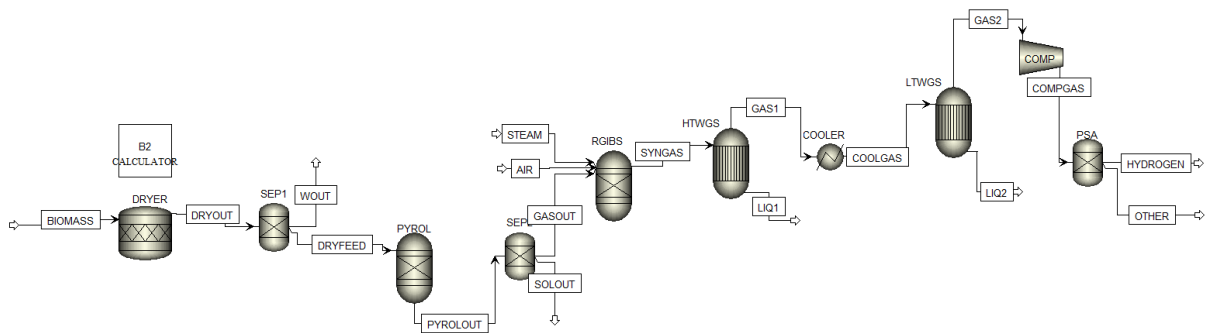


Fig. 2: Aspen Plus flow chart of the system.

Gasification module

The BIOMASS 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 1. Drying occurs at 150 °C to achieve the moisture reduction to 5 wt.% of the original sample. This step is directed by the stoichiometric reactor RSTOIC in the Aspen Plus. This particular module is used to perform chemical reactions of known stoichiometry [42]. After drying, RYIELD, the yield reactor is brought to simulate the feed pyrolysis. In this step, the feedstock is converted to volatile materials (VM) and char. VM contains 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. Then RGibbs is used to simulate the biomass gasification. The decomposed feed, and gasifying agent (air or air-steam) enter to the RGibbs reactor where partial oxidation and gasification reactions occur. The reactor calculates the syngas composition by minimizing the Gibbs free energy and assumes complete chemical equilibrium [56].

Water-gas shift module

For this part, two water-gas shift reactors were considered because W-G shift reaction is moderately exothermic, and it tends to shift to the left side at high temperature. One at higher temperature (HTWGS) and the other at lower temperature (LTWGS). In the HTWGS reactor, there is a first low conversion of CO with quick kinetics, but it is not possible to go beyond the equilibrium curve, thus the LTWGS reactor was used [57]. 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 Requil reactors, respectively [28]. Requil is equilibrium reactor for which the chemical and phase equilibrium are determined by stoichiometric calculations.

Separation unit module

In order to reach a high purity of hydrogen, a PSA unit is applied [58,59]. A separation efficiency of 70% for hydrogen and an input pressure of 7 bar for simulation of PSA were considered from the optimal values found in the literature [60-63]. Pressurization was achieved with a compressor, COMP in Fig. 2, before the PSA. The PSA outlet stream, denoted as HYDROGEN in Fig. 2.

Methodology

The developed model for waste biomass gasification integrated W-G shift and separation unit for hydrogen production is used to investigate the gasification performance of timber and wood waste as a lignocellulosic biomass. The effect of gasifier temperature, and steam to biomass ration (SBR) on syngas composition, lower heating value (LHV) of produced gas, hydrogen production efficiency (HPE) and the amount of hydrogen production are investigated. The lower heating value of product gas is calculated as [22,64]:

$$LHV_{\text{syngas}} \left(\frac{KJ}{Nm^3} \right) = 4.2 \times (30 \times y_{CO} + 25.7 \times y_{H_2} + 85.4 \times y_{CH_4}) \quad (2)$$

where y is the mole fraction of gas species in the syngas (dry basis) that can be extracted from the simulation results.

The hydrogen production efficiency (HPE) is an important index to account for the performance of biomass gasification for H_2 production that it is calculated by using equation (3):

$$HPE(\%) = \frac{m_{H_2} \times LHV_{H_2}}{m_{Biomass} \times HHV_{Biomass}} \times 100 \quad (3)$$

Where m_{H_2} is the mass flow rate of hydrogen (kg/hr) that comes from the simulation results, LHV_{H_2} is lower heating value of hydrogen that is 120.1 MJ/kg, $m_{Biomass}$ is the mass flow rate of input biomass (kg/hr), $HHV_{Biomass}$ is the higher heating value of the biomass (MJ/kg); It is calculated by using the following equation [38,65]:

$$HHV_{\text{fuel}} \left(\frac{MJ}{kg} \right) = 0.312 \times (FC) + 0.1534 \times (VM) \quad (4)$$

According to the equation (4), heating value is a function of weight fractions of fixed carbon and volatile matter in the dry and ash-free conditions.

Specific mass flow rate of the produced hydrogen (*SHP*) is the ratio of the mass flow rate of the product hydrogen per mass flow rate of the entering biomass into the system, calculated as below:

$$SHP = \frac{m_{H_2}^i (kg / hr)}{m_{biomass}^i (kg / hr)} \quad (5)$$

Validation

To validate the developed simulation model, the syngas compositions gained from ASPEN simulations were compared with the experimental results of Jayah et al., [66]. In their work, rubber wood was fed 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 taken into account and the comparisons of CO₂, H₂, CO, and N₂ concentrations are shown in Fig. 3. It can be seen that the present model shows very great agreement with the experimental results. The deviation of the model results from experimental values is quantified by mean absolute error that is around 6.5% for all data.

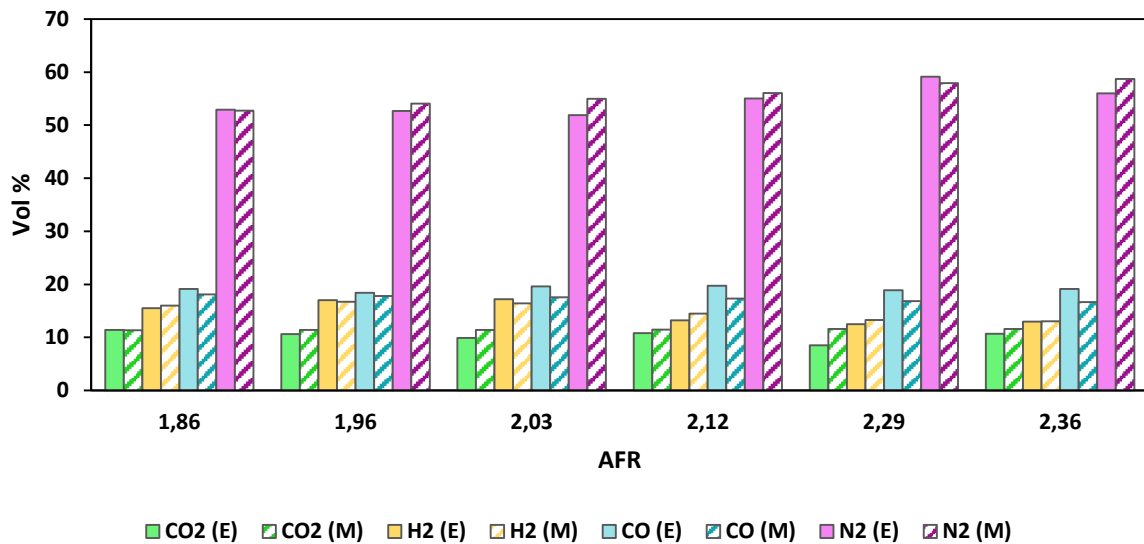


Fig. 3: Comparison of CO₂, H₂, CO, and N₂ concentrations between the simulation model (M) and experimental results (E)

Results and discussion

Effect of temperature on gasification performance and hydrogen production

At the first of this part the effects of the gasification temperature on the syngas compositions under different gasifying agents of air and mixing of air-steam are investigated. In fact, syngas compositions in the form of molar flow rates are evaluated. Temperature varies in the span of 500 to 1500 °C, while the mass flow rate of air to fuel ratio (AFR), steam to biomass ratio (SBR) and biomass feeding rate are fixed at points of 1.8, 0.4, and 1000 kg/hr, respectively. The considered range of 500 to 1500 °C for temperature is based on different literatures focusing

on biomass gasification [23,67,68] as well as our previous works that were properly confirmed and evaluated [27,38,41]. Moreover, 1.8 was considered as AFR for the gasification system derived by timber and wood waste (T&WW) since this value is the optimal AFR for this biomass. This matter has been studied and proved in our pervious works [27,39]. The selection of 0.4 as a fixed point through the temperature analysis is also based on the research work conducted by Marcantonio et al., (2019) [28].

The variation of molar flow rate of syngas and its compositions by increasing temperature under two agents of air and air-steam mixture, were shown in Fig. 4 and Fig. 5, respectively. For both systems by growing the gasifier temperature, H₂ and CO flow rates are also increased. However, in such this condition, the flow rates of CO₂ and CH₄ show a reverse trend. Moreover, growth of the flow rates of CO and H₂ in the range of 500 to 800 °C is because of the combined effect of boudouard, steam methane reforming and water-gas reaction. These are endothermic reactions in nature, hence they are favored with higher temperature. Obviously, H₂ flow rate lessens after 800 °C that it can be attributed to the combined effect of all the reactions occurring in the reduction zone. At low temperatures, water gas shift reaction contributed to hydrogen production, but this reaction was hindered at high temperatures.

In fact, at the higher temperature, the reactions of water gas shift and steam methane reforming contribute majorly to H₂ production. However, the steam methane reforming reaction is limited due to the absence of CH₄ as the main reactant. Therefore, it can be concluded that water gas shift reaction mainly controls the H₂ production.

Furthermore, reduction in CO₂ flow rate by increasing of temperature is due to the boudouard reaction which utilizes CO₂ to produce CO and it is endothermic in nature that is favored at higher temperatures. Methane is also produced through the methanation reaction that is an exothermic reaction and it is favored at lower temperatures. Thus, decrease in CH₄ flow rate is observed when the temperature is increased.

Referring to Fig. 5, the value of hydrogen product from the system derived by air-steam agent is at the highest statues for all studied temperatures. It can be also observed that over the temperature range of 800-1500 °C, the hydrogen production by applying the air-steam based gasification decreases from a maximum value of 44.3 to 38.3 Kmol/hr. Moreover, this indicator for the air based system decreases from 34.4 to 33.7 Kmol/hr.

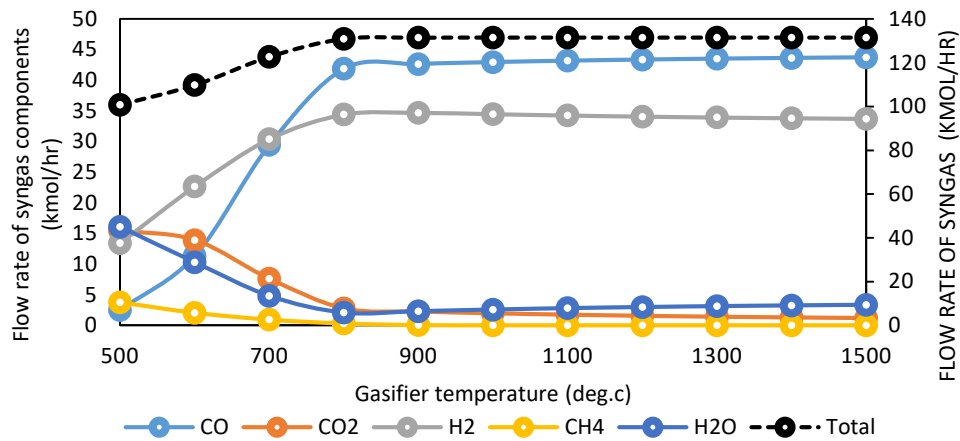


Fig. 4: Effect of gasification temperature on molar flow rates of syngas constituents- air is only gasifying agent.

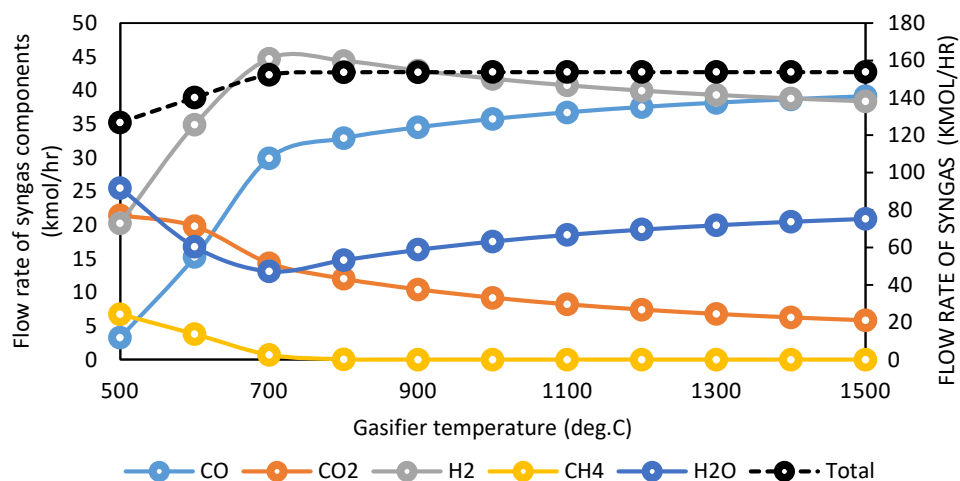


Fig. 5: Effect of gasification temperature on molar flow rates of syngas constituents- mixing of air-steam is gasifying agent.

The variation of the syngas LHV by increasing of the gasification temperature under two gasifying agents were drawn in Fig. 6. Abruptly, LHV increases from 3.7 to 7.05 MJ/Nm³ in span of 500 to 800 °C for the air-based system. The increasing trend of this factor for air-steam gasifications is from 4.9 to 6.3MJ/Nm³ in temperature range of 500 to 700 °C. However, for both conditions it almost became constant. At lower temperatures (500-700 °C), syngas LHV obtained from the air-steam gasification is much higher than the air gasification. However, by increasing the temperature, this indicator for the air agent based system goes upper than the system derived by air-steam agent. This is due to the sum of hydrogen and carbon monoxide content is mainly responsible for the LHV value of the syngas. According to equation (2), the LHV of syngas is function of H₂, CO, and CH₄ mole fractions, so it increases till 700 °C because of the increase in H₂, CO, and CH₄ concentrations. After 700 °C, LHV does not show so much variation due to decreasing in H₂ concentration and slightly increasing of CO concentration.

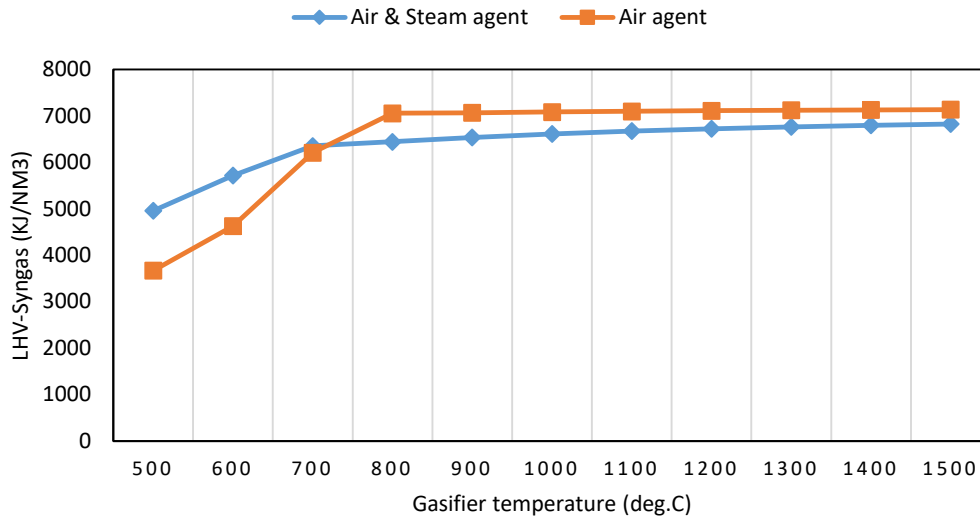


Fig. 6: Effect of gasification temperature on syngas LHV under two different agents.

At the next step, the effect of the gasifier temperature on the hydrogen production efficiency (HPE) and the specific mass flow rate of hydrogen production (SHP) are evaluated. The results of this part based on the functional unit of 1000 kg/hr from timber and wood waste entering to the system have been brought in Fig. 7 and Fig. 8.

As the gasifier temperature is grown (till 800 °C), the syngas production is also increased; then it approximately became constant. Hydrogen production also follows such this trend since it is affected mainly by the input syngas to its process. Fig. 7 reveals that, the HPE values by the air-steam gasification show the highest statuses for all the studied temperatures. HPE is also maximum for both systems over the temperature of 800°C, it values 54 and 33% for the air-steam gasification and the air based system, respectively. Moreover, Fig. 8 shows the process of the air-steam gasification yields 33 kg/hr hydrogen product from 1000 kg/hr timber and wood waste at 500 °C, then it can be increased to 83 kg/hr at 800 °C. However, the SHP for the gasification based on only air agent varies from 0.022 to 0.052 kg_{hydrogen}/kg_{T&WW} in the considered range of temperature.

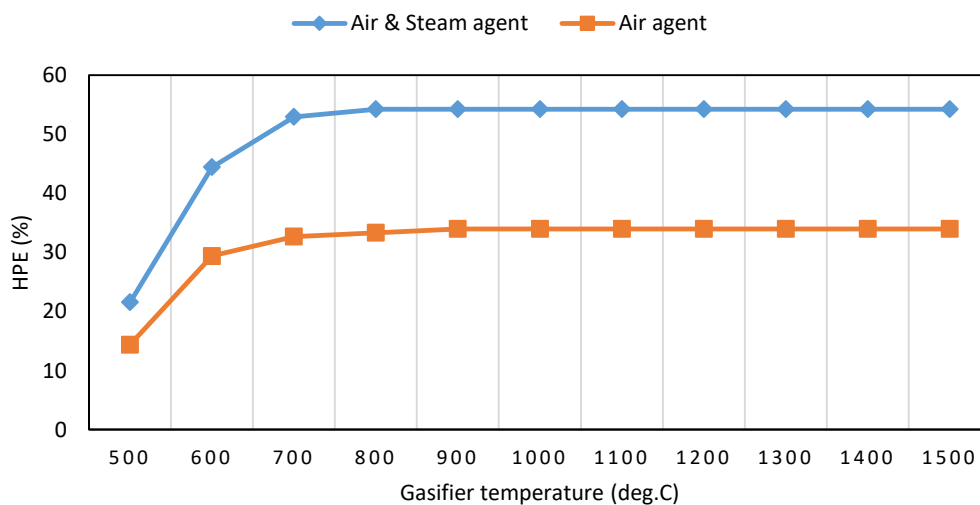


Fig. 7: Effect of gasification temperature on hydrogen production efficiency.

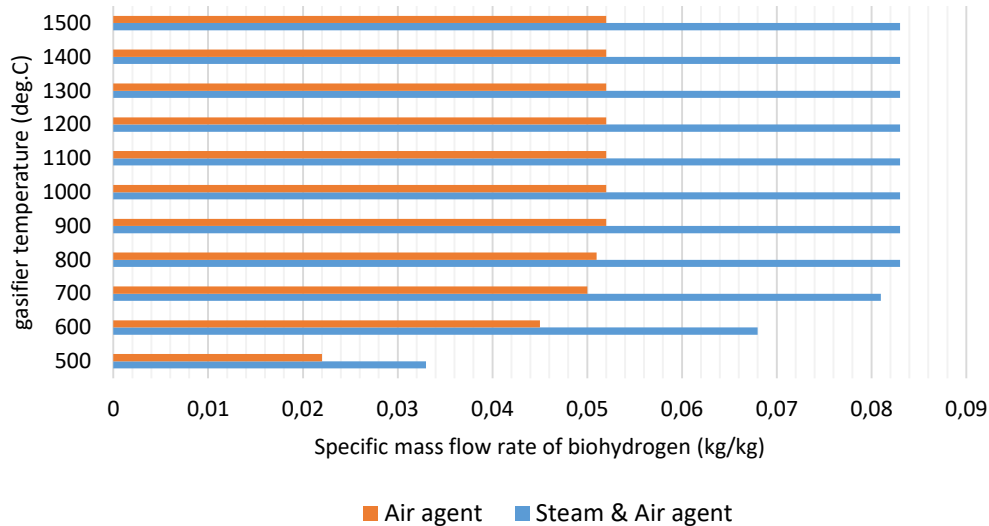


Fig. 8: Effect of gasification temperature on specific mass flow rate of hydrogen production.

Effect of SBR on gasification performance and hydrogen production

In this part, the effect of steam injection on syngas production is studied. It is assumed that the gasifier temperature is set on 800 °C and steam at 150 °C and 1 bar is injected to the system. The steam to biomass ratio (SBR) is varied from 0.1-0.9 and the result is shown in Fig. 9. The overall behavior is that the molar flow rates of H₂ and CO₂ are increased with steam injection and that of CO decreases. This can be explained due to water gas reaction; steam injection leads to rise in the molar flow rate of H₂ and CO in the syngas but stand on the CO shift reaction, the amount of H₂ is increased further and that of carbon monoxide decreases.

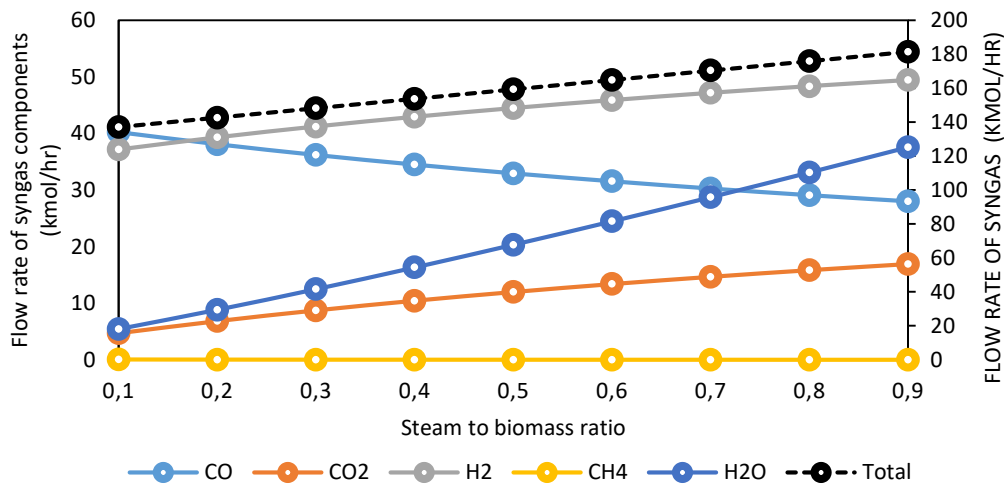


Fig. 9: Effect of SBR on molar flow rates of syngas constituents.

The effects of SBR on syngas LHV and hydrogen production efficiency were shown in Fig. 10. It can be observed that LHV of syngas decreases from 6.9 MJ/Nm³ at SBR = 0.1 to 6.15 MJ/Nm³ at SBR = 0.9. It was explained that by increasing steam injection, the CO production in syngas is moved down due to the water gas shift reaction, so the heating value of the syngas is reduced. Moreover, due to the W-G shift reaction, H₂ production in the product gas is grown

but its degree of increase is not enough that can cover impact of the degree of CO reduction. Referring to Fig. 10, hydrogen production efficiency raises, stemming from the growth of H₂. It values 39.2% at SBR = 0.1 that grows to 70% at SBR = 0.9.

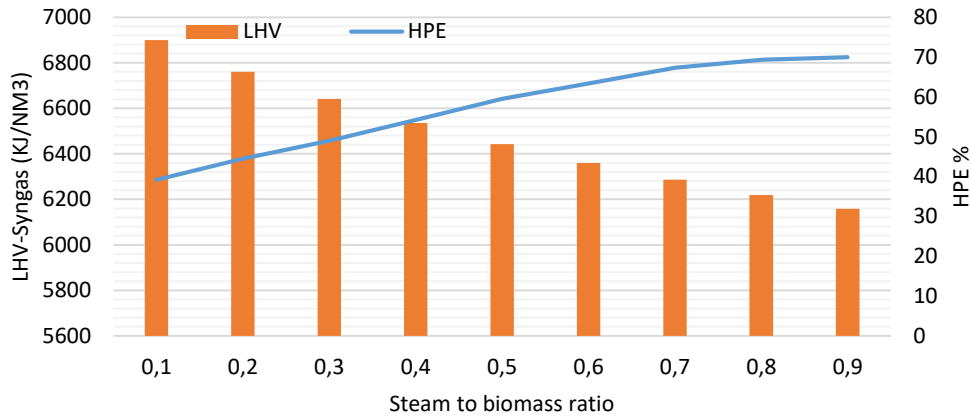


Fig. 10: Effect of SBR on syngas LHV and HPE.

Fig. 11 depicts the effect of the steam to biomass ratio on the specific mass flow rate of hydrogen production from timber and wood waste. As it can be seen, at lower SBR, the flow rate of hydrogen increases with a greater slope and then reaches to almost flatter shape. Hence, it is interesting to find the appropriate range of SBR for biomass gasification integrated with hydrogen production that has been studied in this work. As shown in Fig. 11 the optimum SBR lies between 0.7-0.8 that specific mass flow rate of hydrogen is higher than 0.1 kg_{hydrogen}/kg_{T&WW}.

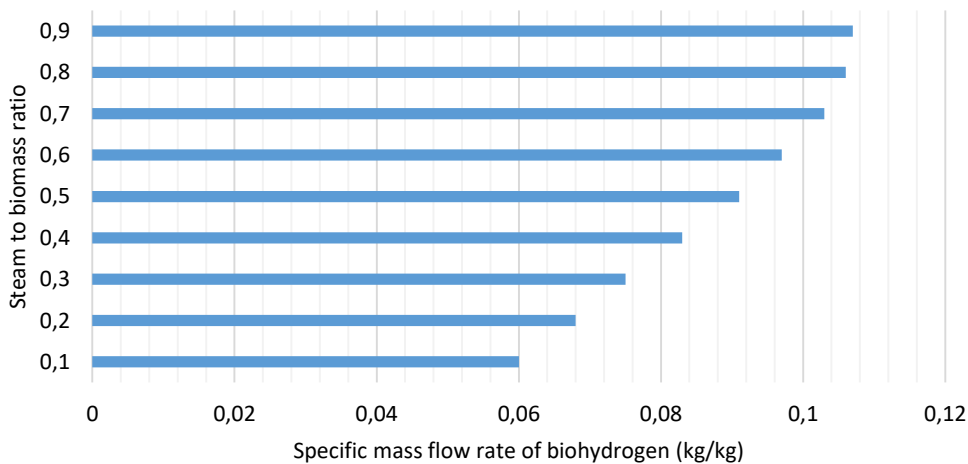


Fig. 11: Effect of SBR on specific mass flow rate of hydrogen production.

Conclusions

In this study, a simulation model by using ASPEN Plus was developed for the gasification integrated with water-gas shift reactors and separation unit for hydrogen production. Timber and wood waste as a lignocellulosic biomass was also considered as the input feedstock to the system. Then, the model was applied to investigate the effect of two agents of air and a mixture of air and steam under different operating conditions of temperature and steam to biomass ratio (SBR) on the gasification performance and hydrogen production.

The results show that the produced hydrogen through the air-steam gasification is at the highest points for all studied temperatures and it would be maximum (44.37 Kmol/hr per 1 ton T&WWs) at 700 °C. At lower temperatures (500-700 °C), the syngas LHV obtained from the air-steam gasification is much higher than the air-based system. However, by increasing temperature, this indicator for the air agent based system goes upper than the system derived by air-steam agent. Moreover, the hydrogen production efficiency (HPE) of the air-steam gasification is at the highest statues for all considered temperatures in comparison to the air-based system. This index would be also maximum around the temperature of 800°C for both systems. It values 54 and 33% for the air-steam gasification and the air gasification, respectively. the process of the air-steam gasification yields 33 kg/hr hydrogen product from 1 ton T&WWs at 500 °C, then it can be increased to 83 kg/hr at 800 °C. However, the specific hydrogen production (SHP) for the air agent gasification varies from 0.022 to 0.052 $\text{kg}_{\text{hydrogen}}/\text{kg}_{\text{T\&WW}}$ in the considered range of temperature.

The LHV of the syngas product decreases from 6.9 Mj/Nm^3 at SBR = 0.1 to 6.15 Mj/Nm^3 at SBR = 0.9. It was explained that by increasing steam injection, the CO production in syngas is moved down due to the water gas shift reaction, so the heating value of the syngas is reduced. Furthermore, the hydrogen production efficiency can be raised, stemming from the growth of H_2 . It values 39.2% at SBR = 0.1 that grows to 70% at SBR = 0.9. The optimum SBR lies between 0.7-0.8 that specific mass flow rate of hydrogen would be higher than 0.1 $\text{kg}_{\text{hydrogen}}/\text{kg}_{\text{T\&WW}}$.

Acknowledgements

This paper was a part of the project funded by Icelandic Research Fund (IRF), (in Icelandic: Rannsóknasjóður) and the grant number is 196458-051.

Conflicts of Interest: The authors declare no conflicts of interest

References

1. Safarian S, Khodaparast P, Kateb M. Modeling and technical-economic optimization of electricity supply network by three photovoltaic systems. *Journal of Solar Energy Engineering*. 2014;136(2):024501.
2. Rajaeifar MA, Akram A, Ghobadian B, et al. Environmental impact assessment of olive pomace oil biodiesel production and consumption: A comparative lifecycle assessment. *Energy*. 2016;106:87-102.

3. Talebnia F, Karakashev D, Angelidaki I. Production of bioethanol from wheat straw: an overview on pretreatment, hydrolysis and fermentation. *Bioresource technology*. 2010;101(13):4744-4753.
4. Safarian S, Unnthorsson R, Richter C. Techno-Economic Analysis of Power Production by Using Waste Biomass Gasification. *Journal of Power and Energy Engineering*. 2020;8(06):1.
5. Sarıdemir S, Ağbulut Ü. Combustion, performance, vibration and noise characteristics of cottonseed methyl ester–diesel blends fuelled engine. *Biofuels*. 2019:1-10.
6. Zeng J, Xiao R, Zhang H, et al. Chemical looping pyrolysis-gasification of biomass for high H₂/CO syngas production. *Fuel Processing Technology*. 2017;168:116-122.
7. Luo H, Lin W, Song W, et al. Three dimensional full-loop CFD simulation of hydrodynamics in a pilot-scale dual fluidized bed system for biomass gasification. *Fuel Processing Technology*. 2019;195:106146.
8. Kumar B, Bhardwaj N, Agrawal K, et al. Current perspective on pretreatment technologies using lignocellulosic biomass: An emerging biorefinery concept. *Fuel Processing Technology*. 2020;199:106244.
9. Ahmadi P, Dincer I, Rosen MA. Development and assessment of an integrated biomass-based multi-generation energy system. *Energy*. 2013;56:155-166.
10. Shayan E, Zare V, Mirzaee I. Hydrogen production from biomass gasification; a theoretical comparison of using different gasification agents. *Energy Conversion and management*. 2018;159:30-41.
11. Yue G, Zhang H, Zhao C, et al. *Proceedings of the 20th International Conference on Fluidized Bed Combustion*. Springer Science & Business Media; 2010.
12. Di Carlo A, Borello D, Bocci E. Process simulation of a hybrid SOFC/mGT and enriched air/steam fluidized bed gasifier power plant. *International Journal of Hydrogen Energy*. 2013;38(14):5857-5874.
13. Cherubini F, Peters GP, Berntsen T, et al. CO₂ emissions from biomass combustion for bioenergy: atmospheric decay and contribution to global warming. *Gcb Bioenergy*. 2011;3(5):413-426.
14. Huda A, Mekhilef S, Ahsan A. Biomass energy in Bangladesh: Current status and prospects. *Renewable and Sustainable Energy Reviews*. 2014;30:504-517.
15. Safarian S, Unnthorsson R, Richter C. A review of biomass gasification modelling. *Renewable and Sustainable Energy Reviews*. 2019;110:378-391.
16. Safarian S, Sattari S, Hamidzadeh Z. Sustainability assessment of biodiesel supply chain from various biomasses and conversion technologies. *BioPhysical Economics and Resource Quality*. 2018;3(2):6.
17. Safarian S, Sattari S, Unnthorsson R, et al. Prioritization of Bioethanol Production Systems from Agricultural and Waste Agricultural Biomass Using Multi-criteria Decision Making. *Biophysical Economics and Resource Quality*. 2019;4(1):4.
18. Safarian S, Unnthorsson R. An assessment of the sustainability of lignocellulosic bioethanol production from wastes in Iceland. *Energies*. 2018;11(6):1493.
19. Inayat A, Raza M, Khan Z, et al. Flowsheet Modeling and Simulation of Biomass Steam Gasification for Hydrogen Production. *Chemical Engineering & Technology*. 2020;43(4):649-660.
20. Safarian S, Ebrahimi Saryazdi SM, Unnthorsson R, et al. Artificial neural network integrated with thermodynamic equilibrium modeling of downdraft biomass gasification-power production plant. *Energy*. 2020:118800.
21. Safarian S, Unnthorsson R, Richter C. The equivalence of stoichiometric and non-stoichiometric methods for modeling gasification and other reaction equilibria. *Renewable and Sustainable Energy Reviews*. 2020;131:109982.
22. Kuo P-C, Wu W, Chen W-H. Gasification performances of raw and torrefied biomass in a downdraft fixed bed gasifier using thermodynamic analysis. *Fuel*. 2014;117:1231-1241.

23. Ramzan N, Ashraf A, Naveed S, et al. Simulation of hybrid biomass gasification using Aspen plus: A comparative performance analysis for food, municipal solid and poultry waste. *Biomass and bioenergy*. 2011;35(9):3962-3969.
24. Gordillo G, Annamalai K, Carlin N. Adiabatic fixed-bed gasification of coal, dairy biomass, and feedlot biomass using an air–steam mixture as an oxidizing agent. *Renewable Energy*. 2009;34(12):2789-2797.
25. All Power Laboratories Berkeley, CA: APL; 2012. Available from: <http://www.allpowerlabs.com/>
26. Safarian S, Unnthorsson R, Richter C. Simulation and Performance Analysis of Integrated Gasification–Syngas Fermentation Plant for Lignocellulosic Ethanol Production. *Fermentation*. 2020;6(3):68.
27. Safarian S, Unnthorsson R, Richter C. Performance analysis and environmental assessment of small-scale waste biomass gasification integrated CHP in Iceland. *Energy*. 2021:117268.
28. Marcantonio V, De Falco M, Capocelli M, et al. Process analysis of hydrogen production from biomass gasification in fluidized bed reactor with different separation systems. *International Journal of Hydrogen Energy*. 2019;44(21):10350-10360.
29. Balat H, Kirtay E. Hydrogen from biomass–present scenario and future prospects. *International Journal of Hydrogen Energy*. 2010;35(14):7416-7426.
30. Martin M, Svensson N, Fonseca J, et al. Quantifying the environmental performance of integrated bioethanol and biogas production. *Renewable energy*. 2014;61:109-116.
31. Yoon SJ, Son Y-I, Kim Y-K, et al. Gasification and power generation characteristics of rice husk and rice husk pellet using a downdraft fixed-bed gasifier. *Renewable Energy*. 2012;42:163-167.
32. Safarian S, Saboohi Y, Kateb M. Evaluation of energy recovery and potential of hydrogen production in Iranian natural gas transmission network. *Energy policy*. 2013;61:65-77.
33. Çağlar A, Demirbaş A. Hydrogen rich gas mixture from olive husk via pyrolysis. *Energy Conversion and Management*. 2002;43(1):109-117.
34. Frigo S, Spazzafumo G. Cogeneration of power and substitute of natural gas using biomass and electrolytic hydrogen. *International Journal of Hydrogen Energy*. 2018;43(26):11696-11705.
35. Li Q, Song G, Xiao J, et al. Exergy analysis of biomass staged-gasification for hydrogen-rich syngas. *International Journal of Hydrogen Energy*. 2019;44(5):2569-2579.
36. Jin H, Fan C, Wei W, et al. Evolution of pore structure and produced gases of Zhundong coal particle during gasification in supercritical water. *The Journal of Supercritical Fluids*. 2018;136:102-109.
37. Omar MM, Munir A, Ahmad M, et al. Downdraft gasifier structure and process improvement for high quality and quantity producer gas production. *Journal of the Energy Institute*. 2018;91(6):1034-1044.
38. Safarian S, Richter C, Unnthorsson R. Waste Biomass Gasification Simulation Using Aspen Plus: Performance Evaluation of Wood Chips, Sawdust and Mixed Paper Wastes. *Journal of Power and Energy Engineering*. 2019;7(6):12-30.
39. Safarian S, Unnthorsson R, Richter C. Simulation of small-scale waste biomass gasification integrated power production: a comparative performance analysis for timber and wood waste. *International Journal of Applied Power Engineering (IJAPE)* 2020;09(02):147-152.
40. Safarian S, Unnthorsson R, Richter C. Techno-economic and environmental assessment of power supply chain by using waste biomass gasification in Iceland. *BioPhysical Economics and Sustainability*. 2020;5:7.
41. Safarianbana S, Unnthorsson R, Richter C, editors. Development of a new stoichiometric equilibrium-based model for wood chips and mixed paper wastes gasification by ASPEN Plus. *ASME International Mechanical Engineering Congress and Exposition; 2019: American Society of Mechanical Engineers*.
42. Damartzis T, Michailos S, Zabaniotou A. Energetic assessment of a combined heat and power integrated biomass gasification–internal combustion engine system by using Aspen Plus®. *Fuel processing technology*. 2012;95:37-44.

43. Kobayashi N, Tanaka M, Piao G, et al. High temperature air-blown woody biomass gasification model for the estimation of an entrained down-flow gasifier. *Waste Management*. 2009;29(1):245-251.
44. Nguyen TLT, Hermansen JE, Nielsen RG. Environmental assessment of gasification technology for biomass conversion to energy in comparison with other alternatives: the case of wheat straw. *Journal of cleaner production*. 2013;53:138-148.
45. Porcu A, Sollai S, Marotto D, et al. Techno-Economic Analysis of a Small-Scale Biomass-to-Energy BFB Gasification-Based System. *Energies*. 2019;12(3):494.
46. Roy D, Samanta S, Ghosh S. Thermo-economic assessment of biomass gasification-based power generation system consists of solid oxide fuel cell, supercritical carbon dioxide cycle and indirectly heated air turbine. *Clean Technologies and Environmental Policy*. 2019;21(4):827-845.
47. Gil J, Corella J, Aznar MaP, et al. Biomass gasification in atmospheric and bubbling fluidized bed: effect of the type of gasifying agent on the product distribution. *Biomass and bioenergy*. 1999;17(5):389-403.
48. Meramo-Hurtado SI, Puello P, Cabarcas A. Process Analysis of Hydrogen Production via Biomass Gasification under Computer-Aided Safety and Environmental Assessments. *ACS omega*. 2020;5(31):19667-19681.
49. Nakyai T, Authayanun S, Patcharavorachot Y, et al. Exergoeconomics of hydrogen production from biomass air-steam gasification with methane co-feeding. *Energy Conversion and Management*. 2017;140:228-239.
50. Basu P. *Combustion and gasification in fluidized beds*. CRC press; 2006.
51. Boerrigter H, Rauch R. Review of applications of gases from biomass gasification. *ECN Biomassa, Kolen en Milieuonderzoek*. 2006;20.
52. Puig-Arnavat M, Bruno JC, Coronas A. Review and analysis of biomass gasification models. *Renewable and Sustainable Energy Reviews*. 2010;14(9):2841-2851.
53. Moneti M, Di Carlo A, Bocci E, et al. Influence of the main gasifier parameters on a real system for hydrogen production from biomass. *International Journal of Hydrogen Energy*. 2016;41(28):11965-11973.
54. Safarian S, Bararzadeh M. Exergy analysis of high-performance cycles for gas turbine with air-bottoming. *Journal of Mechanical Engineering Research*. 2012;5(2):38-49.
55. Adeniyi AG, Ighalo JO, Amosa MK. Modelling and simulation of banana (*Musa spp.*) waste pyrolysis for bio-oil production. *Biofuels*. 2019:1-5.
56. Tauqir W, Zubair M, Nazir H. Parametric analysis of a steady state equilibrium-based biomass gasification model for syngas and biochar production and heat generation. *Energy Conversion and Management*. 2019;199:111954.
57. Preciado JE, Ortiz-Martinez JJ, Gonzalez-Rivera JC, et al. Simulation of synthesis gas production from steam oxygen gasification of Colombian coal using Aspen Plus®. *Energies*. 2012;5(12):4924-4940.
58. Sjardin M, Damen K, Faaij A. Techno-economic prospects of small-scale membrane reactors in a future hydrogen-fuelled transportation sector. *Energy*. 2006;31(14):2523-2555.
59. Li A, Liang W, Hughes R. The effect of carbon monoxide and steam on the hydrogen permeability of a Pd/stainless steel membrane. *Journal of Membrane Science*. 2000;165(1):135-141.
60. Carrara A, Perdichizzi A, Barigozzi G. Simulation of an hydrogen production steam reforming industrial plant for energetic performance prediction. *International journal of hydrogen energy*. 2010;35(8):3499-3508.
61. Sircar S, Waldron WE, Anand M, et al. Hydrogen recovery by pressure swing adsorption integrated with adsorbent membranes. *Google Patents*; 1998.
62. Pallozzi V, Di Carlo A, Bocci E, et al. Performance evaluation at different process parameters of an innovative prototype of biomass gasification system aimed to hydrogen production. *Energy Conversion and Management*. 2016;130:34-43.

63. Honeywell U. Years of PSA Technology for H₂ Purification. 2016.
64. Lv P, Xiong Z, Chang J, et al. An experimental study on biomass air–steam gasification in a fluidized bed. *Bioresource technology*. 2004;95(1):95-101.
65. Demirbaş A. Calculation of higher heating values of biomass fuels. *Fuel*. 1997;76(5):431-434.
66. Jayah T, Aye L, Fuller RJ, et al. Computer simulation of a downdraft wood gasifier for tea drying. *Biomass and Bioenergy*. 2003;25(4):459-469.
67. Dahmani M, Périlhion C, Marvillet C, et al., editors. Development of a fixed bed gasifier model and optimal operating conditions determination. *AIP Conference Proceedings*; 2017: AIP Publishing LLC.
68. Doherty W, Reynolds A, Kennedy D. Simulation of a circulating fluidised bed biomass gasifier using ASPEN Plus: a performance analysis. 2008.