

## Model development and energy and exergy analysis of the biomass gasification process (Based on the various biomass sources)



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### ABSTRACT

Worldwide growing demand for energy consumption in recent years arising from industrialization development and increasing earth population has caused more environmental concerns to emerge. On the other hand, specific issues related to the use of fossil fuels as a nonrenewable source of energy has been caused alternative fuels like biomass to be investigated with more concern. Generally, gasification is a process which converts organic matter to gas and tar. Also, through the gasification, biomass as a fuel is converted to the combustible gas (syngas). In this study, modeling and simulation of the biomass gasification process is investigated and analyzed considering 23 different kinds of the biomass sources. The proposed model is based on the Gibbs free energy minimization and the restricted equilibrium method is used for calibration. The process operating performance is analyzed thermodynamically based on the hydrogen production yield. In this regard, effective parameters like temperature of the gasification, air-fuel ratio, steam-biomass ratio and temperature of the air and steam streams are investigated. Gasification temperature and steam-biomass ratio affect the syngas compositions and the heating value significantly. Biomass moisture has the most significant impact on the syngas production efficiency. Also, other parameters which are not very intensive but still have an effect on the syngas production efficiency, are examined. Finally, the process performance is analyzed based on the energy and exergy analysis methods. The obtained results show that, exergy efficiency of drying stage is the highest (about 90.0%) in all cases. Nonetheless, exergy destruction rate for this stage is a great value against the others. Among the selected biomasses, Rice husk type has the greatest exergy destruction rate which is related to the tar combustion and decomposition reactors; respectively.

### 1. Introduction

After coal and oil, biomass as a renewable source is one of the largest sources of energy that is extracted from the organic materials and natural resources [1]. Biomass includes a wide range of materials that agricultural residue and forest residue have the biggest portion in it. Agriculture residues are from resources such as husk, bagasse, straw and forest residues are like bark, sawdust and wood chips [2,3]. Municipal solid wastes is another source of biomass fuel. Depending on the potentiality of different countries, variety range of different biomass sources are known as the renewable resources for fuel production. Because the net carbon dioxide (CO<sub>2</sub>) emission from the biomass is zero, so it is quite clean in comparison with other sources of energy. In the thermochemical gasification process, CO<sub>2</sub> is one of the emission

gaseous while in the biomass gasification, CO<sub>2</sub> is consumed by biomass in the photosynthesis process [4]. Hydrogen (H<sub>2</sub>) is known as an effective and clean fuel for the fuel cells and combustion engines. Biomass is one of the important resources to produce hydrogen and biofuel. Different method have been produced for production of Hydrogen. Steam reforming of the natural gas, water (H<sub>2</sub>O) electrolysis and coal gasification are of the most common methods. But they are not known as a sustainable procedure to produce hydrogen, because electricity or fossil fuels are gained from the non-renewable sources. Gasification and pyrolysis, as alternative thermochemical method and bio-photolysis, water-gas shift reaction and fermentation as biological method are more sustainable than conventional methods [5,6]. Several researches have been conducted regarding the technologies of hydrogen production from the biomass [7–9]. One of the most important sections of

*Abbreviations:* C, Carbon; CO<sub>2</sub>, Carbon dioxide; CO, Carbon monoxide; CH<sub>4</sub>, Methane; CCHP, Combined cooling, heat and power; E, Heat Exchanger; H<sub>2</sub>, Hydrogen; H<sub>2</sub>O, Water; H<sub>2</sub>S, Hydrogen sulfide; N<sub>2</sub>, Nitrogen; NH<sub>3</sub>, Ammonia; NO<sub>2</sub>, Nitrogen dioxide; O<sub>2</sub>, Oxygen; S, Sulfur; SO<sub>2</sub>, Sulfur dioxide; SOFC, Solid oxy fuel cell

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Nomenclature			
$a_1, \dots, a_6$	Coefficients in entropy equation [dimensionless]	x	Thickness [m]
A	Gasifier area in $m^2$ or pre-exponential constant [ $s^{-1}$ or $min^{-1}$ ]	$U_0$	Wind velocity [m/s]
C	Carbon content in biomass [wt%]	<b>Greek letters</b>	
$C_p$	Specific heat capacity at constant pressure [kJ/kg °C]	$\eta$	Efficiency [-]
E	Activation energy [kJ mol $^{-1}$ ]	$\beta$	Coefficient
$\dot{E}$	Energy flow rate [kJ/h]	$\varepsilon$	Gasifier wall emissivity [-]
Ex	Exergy [kJ/kg or kJ/kmol]	<b>Subscripts</b>	
$Ex_0$	Standard exergy [kJ/kmol]	BCL	Battelle Columbus Laboratory
$\dot{E}x$	Exergy rate [kW]	ch	Chemical
h	Specific enthalpy [kJ/kg or kJ/kmol]	cg	Syngas
H	Hydrogen content in biomass (wt%) or total enthalpy [kJ]	des	Exergy destroyed
$\dot{I}$	Irreversibility [kW]	deswa	Exergy loss
k	Rate constant or kinetic constant [ $s^{-1}$ ]	drybio	Dry biomass
LHV	Lower heating value [kJ/kg or kJ/kmol]	e	Exit
$\dot{m}$	Mass flow rate [kg/s]	En	Energy
MW	Molecular weight [kg/kmol]	gen	Generation
N	Nitrogen content in biomass [wt%]	i	Inlet or Component “i”
O	Oxygen content in biomass [wt%]	ins	Insulation
P	Pressure or partial pressure [Pa or atm]	j	Component “j”
PI	Improvement potential [kW]	lostwa	Lost from gasifier wall to ambient
Q	Heat transferred to ambient [kW]	o	At reference or ambient or outlet
R	Universal gas constant [8.314 KJ/kmol K]	ph	Physical
T	Gasification temperature [K]	prodg	Produced gas
$T_0$	Reference temperature [298 K]	P	Number of products
s	Specific entropy [KJ/kmo K or KJ/kg K]	R	Number of reactants
$\dot{s}$	Entropy [kW/K]	w	Wall
S	Sulfur content in biomass (wt%) or total entropy [kJ]	wa	From gasifier wall to ambient
t	Time [s]		
$\dot{W}$	Electrical power [W or kW]		
X	Molar fraction of component [dimensionless]		

hydrogen production is gasifier that has been investigated so much [5,6]. In different studies, Aspen plus process simulator has been used to investigate and simulate the coal conversion in different processes like methanol synthesis, integrated coal gasification combined cycle power plants [3], coal hydro-gasification process and simulation [10], compartmented fluidized bed coal gasifiers [11], coal hydro-gasification processes [12] and coal gasification simulation [13]. A research is done on biomass gasification [14]. In biomass gasification, gasifier is the main stage of the process. [15]. The gasification, featured with a limited oxidation, can be used in various clean energy processes like hydrogen production via biomass gasification. Gasifier modeling and simulation is done in some researchers by Aspen plus [3,9,16]. Some researchers have claimed that biomass gasification in supercritical  $H_2O$  can be considered as a superior technology in  $H_2$  production [7,8]. In this regard, energy and exergy efficiencies and also operating performance improvement along with data availability with experimental studies [6] have received the most attention in recent studies [17–19].

Various integrated processes have been proposed and analyzed to improve the operating performance efficiency of the biomass gasification process. Kalina et al. [20] presented a mathematical concept model of a small-scale combined electrical power generation cycles integrated with thermal gasification of the biomass. The obtained results show that biomass to electricity conversion efficiency in the best case is at the range of 22.3–37.7%. Taheri et al. [21] proposed a novel integrated multi-generation energy system with hydrogen production from biomass and liquefied natural gas regasification cycle. The process is examined based on the energy, exergy and economic analyses. The results indicate that, with increasing the biomass flow rate as the fuel from 4 kg/s to 10 kg/s, overall energy efficiency decreases 8.50% and total cost rate of the process increases of 123%. Santhanam et al. [22]

evaluated a thermodynamic model of integrated biomass gasification and solid oxide fuel cell (SOFC) and small-scale gas turbine system (100 kWe). Based on the exergy analysis results, highest exergy loss belongs to gasifier, gas turbine and waste heat recovery system respectively. To decrease the exergy losses and increase the system performance efficiency, a new strategy for heat pipe integration is proposed. This development leads to increase the electrical efficiency from 55% to 72% by decreasing exergy losses in the gasifier. Wang et al. [23] analyzed the cost allocation of two integrated structures of the combined cooling, heat and power (CCHP) system based on the modified exergoeconomic method. Moharamian et al. [24] investigate a comparative thermoeconomic evaluation of three biomass and biomass-natural gas-fired combined cycles using organic Rankine cycles. The proposed structures are biomass integrated co-fired, post-firing and externally fired combined cycles. The highest and lowest energy and exergy efficiencies are illustrated by the biomass integrated post-fired (37.0% and 34.0%) and externally fired (36.0% and 21.0%) combined cycles, respectively. Tan et al. [25] analyzed a novel integrated structure of the hybrid system which includes electrical power generation, biomass gasification, SOFC, gas expanders and the Kalina cycle. The performance was evaluated by conducting energy and exergy analyses. The results showed that, the energy efficiency of the hybrid system can reach to 64.2% for the produced syngas lower heating value (LHV) in a system baseline operating condition. Stougje et al. [26] compared the use of livestock manure and verge grass for three different structures of electrical power generation from the biomass by using environmental and an exergetic life cycle assessments. As concluded, the differences between the environmental and exergetic sustainability assessment scores of the systems are not large. Yan et al. [27] thermodynamically analyzed a novel chemical looping electrical power generation system based on the

biomass–coal co-gasification with steam. Energy and exergy efficiencies of the process components were calculated. Yan et al. [28] studied characteristics of a clean electrical power generation system based on the steam co-gasification of biomass and coal. Chemical looping with oxygen uncoupling technology and combination of the SOFC and steam turbine were utilized to supply oxygen and generate electrical power, respectively. Also, CO<sub>2</sub> capture is performed by implementing the calcium looping and mineral carbonation. The obtained results indicate that, the highest value of the energy and exergy losses belongs to the steam turbine. Also, the energy and exergy efficiencies are about 50.0% and 47.0%, respectively. Li et al. [29] presented an exergy and environmental analysis of a novel tri-generation system with biomass gasification and solar thermal energy utilization. The results show that, the solar thermal energy contribution leads to decrease in the biomass consumption rates. Manatura et al. [30] performed an exergy analysis to evaluate the experimental gasification process of torrefied biomass obtained from the rice husk pellets (RHP) as the feedstock. The results show that, the overall energy efficiency decreases because of the energy loss in volatile gas and electrical power consumption in the combined torrefaction-gasification process. Zhang et al. [31] proposed a thermodynamic and economic analysis of biomass partial gasification model based on the principle of cascade utilization of chemical energy. Wherein, the remained parts of the biomass which are not participating in the gasification are utilized as the boiler fuel. The model exergy efficiency can reach to 68.0% by considering both of the biogas and char as products. Also, the initial capital cost saving ratio is about of 13.0% in comparison with complete biomass gasification. Bai et al. [32] proposed thermodynamic performance analysis of a new integrated solar-biomass combined electrical power generation cycle with a two-stage gasifier. The results indicate that, two-stage gasifier configuration has an advantage of 19.3% decrease in exergy loss for the solar thermal energy collection and biomass gasification in comparison with one-stage ones. Wang et al. [33] proposed a hybrid CCHP system driven by biomass and solar energy with complementarity analysis between the biomass and solar energy to enhance the system's energy efficiency. The analysis shows that, the biomass makes a greater contribution to the total system primary energy ratio and exergy efficiency than the solar subsystem. Nakyai et al. [34] investigated effects of various kinds of gasifying agent, (air and both steam and air), with and without methane co-feeding for the biomass gasification by implementing an exergoeconomic analysis. It was concluded that, by using steam and air as agents and methane co-feeding, a higher values of the energy and exergy efficiencies can be achieved. Li et al. [35] numerically studied an integrated novel heating and power co-generation system with biomass partial gasification and ground source heat pump thermodynamic performance. The system proposes better usage of biomass and geothermal energy, where an overall energy efficiency and heat to power ratio of 72.1% and 3.93 can be achieved, respectively. Kuo et al. [36] examined a steam co-gasification CCHP system with the maximum waste heat recovery and Rankine cycle which uses blending coal and biomass as a fuel in terms of energy and exergy efficiency. The raw wood, torrefied wood and coal percentages are analyzed. The results showed that, by utilizing torrefied wood and coal compared to raw wood and coal, 8.43% increase in the total electrical power generation production is achieved. Fan et al. [37] presented a thermodynamic and environmental investigation of a CCHP system with biomass and coal co-fuelled gasification chemical looping combustion. At the best operating conditions of the process, the energy and exergy efficiencies can reach 60.2% and 22.2%, respectively. Baghbanbashi et al. [38] studied two reliable methods for fuel production from biomass including supercritical water gasification and hydrothermal upgrading. In this study, the equilibrium mole fraction is calculated based on the Gibbs free energy minimization method for glucose and cellulose supercritical water gasification and hydrothermal upgrading of wood as the feed biomass. Supercritical water gasification and exergy efficiencies are about 88.3% and 83.6%, respectively. Vakalis et al. [39] introduced a

novel thermodynamic-based method for analyzing two small-scale gasifiers performance by means of exergy, entransy and statistical entropy. In this study, an integrated efficiency index is introduced which makes it possible to compare different kinds of the poly-generative energy systems having different design structures and nature of products. Thallam Thattai et al. [40] developed a thermodynamic model of an integrated biomass co-gasification with large scale (253 MWe) combined coal-based cycle in Netherlands. The model predicts net electrical power output and efficiency of the plant for steam-exploded wood pellets. Gholamian et al. [41] proposed thermodynamic analysis of a CCHP system which uses biomass as the fuel. The system consist of SOFC, double effect absorption refrigeration cycle and heat recovery steam generation (HRSG). The system performances is compared with other similar systems by conducting energy and exergy analyses from the environmental considerations view of points. The results indicate that, the maximum system exergy efficiency is 37.9% with a CO<sub>2</sub> emission rates of 20.4 t/MWh. These values present 49.9% increase in system exergy efficiency and 64.0% decrease in CO<sub>2</sub> emission rates. Cruz et al. [42] evaluated a thermodynamic performance of three bioenergy systems through exergy analysis. The proposed base-case system consists of a biomass gasification, Fischer-Tropsch synthesis and combined power generation cycle. In addition, two other structures for improving performance of the base-case system are considered. Remarkable features of these systems are auto-thermal reforming of a fraction of the Fischer-Tropsch tail gas to increase the fuel yield, and combustion a fraction of the syngas to increase electrical power generation efficiency. The results indicate that, the biomass gasification and electrical power generation sub-systems have 50% and 19–28% share of the overall exergy destruction rates.

Biomass gasification simulation is carried out based on the material and energy balance and chemical equilibrium relations [43]. Since the biomass consists of high amount of volatile material and as well as the complexity of the biomass reaction rate kinetics in the reactors, char gasification is ignored [44]. In this case, the simulation of the biomass gasification is done through this assumption that gasification follows Gibbs equilibrium relations [3].

Many reviews have been proposed about biomass gasification models and related issues. For instance, Shahbaz et al. [45] reviewed the influence of catalysts and catalytic potential of the coal bottom ash in the biomass steam gasification. Ramos et al. [46] reviewed co-gasification and recent developments in waste to- energy conversion. La Villetta et al. [47] reviewed the biomass gasification modeling approaches with emphasis on the stoichiometric method. Correa and Kruse [48] reviewed supercritical water biomass gasification for H<sub>2</sub> production. Dalólio et al. [49] reviewed the poultry litter as biomass energy along with its future perspectives. According to the reviewed studies on the biomass gasification process at different operating conditions; it is necessary to provide a comprehensive study about analyzing the biomass gasification process with the aim of using a variety of biomasses as the fuel. In this study, 23 different types of the biomass sources which are Cedar wood, Wood sawdust, Olive oil residue, Rice husk, Rice straw, Pine sawdust, Spruce wood pellet, Coffee husk, Coffee ground, Larch wood, Grapevine pruning waste, Jute stick, Sugar-cane bagasse, Corn cob, Peach stone, Wheat straw, Cotton stem, Straw, Camphor wood, Beech wood, Switchgrass, Oil Palm Shell and Wood Chip are utilized for investigation. This study is based on the development of a simulation model which is capable of predicting the steady-state performance of an atmospheric gasifier. The products of homogeneous reactions are defined by Gibbs equilibrium relations. The developed simulation model is used for analyzing the effective parameters of the gasification process performance. Among the utilized biomasses, three of the most conventional ones which are Rice husk, Larch wood and Wood chip are chosen for detail examination by energy and exergy analyses.

The main objectives of this study are as follow:

- Developing a comprehensive model of the biomass gasification process for H<sub>2</sub> production.
- Hydrogen production yield investigation for different kinds of the biomasses.
- Process sensitivity analysis and as well as parametric study of the effective parameters on the operating performance.
- Energy and exergy analyses for hydrogen production yield via three selected biomasses

## 2. Biomass sources

The base of biomass fuels is solid carbonaceous materials which are remnant of animals and plants. Generally, the biomass can be categorized into the following groups [50]:

- Waste from food processing operations like the rice milling, the refining of cane sugar, and the canning of vegetables and fruits and as well as waste from the processing wood into lumber, plywood, and pulp.
- Crop debris such as straw and energy crops like fast-growing trees, sugar crops manure from cattle, poultry and hogs.

Bulk density, heating value, moisture content, elemental composition, ash content and volatile matter content are of the important biomass properties. Investigation of different types of biomass and also study effect of operating parameters on the performance of the system are required for the design and operation of the gasifier [51]. Main part of the biomass fuel contains cellulose, lignin and hemi cellulose. Among this components, the cellulose molecular structure has various molecular weights. Molecular weight of the hemi-cellulose is lower than the cellulose and there is no defined molecular structure for hemi-cellulose. Hemi-cellulose has a higher activity and lower thermal stability. The lignin molecular structure is similar to low rank coal. So, lignin extraction from the biomass without taking advantage of a chemical modification is difficult. Characteristics of the gasification process is affected by lignocellulosic biomasses. Because, they have many differences in morphological, chemical and physical properties [52]. The most important parameter in the biomass is its heating value.

From the efficiency and economy aspects, biomasses that having

high heating value play a significant role in more energy recovery and improving the operating performance of the system.

On the other hand, using various kinds of biomass wastes with different composition and heating value is possible by providing reactors with effective heat and mass transfer properties [53,54]. Table 1 shows the Ultimate analysis and LHV of the selected biomass feedstock material.

## 3. Gasification process

Gasification is the process of conversion of a carbon-rich solid fuel into a gaseous fuel in the gasifier that takes place in an environment with specific oxygen (O<sub>2</sub>) amount. The reaction can take place at a medium which can be air, O<sub>2</sub>, subcritical steam or a mixture of them [55]. Heating value of the produced gas in the air blown processes is about of 3–5 MJ/m<sup>3</sup> while in the O<sub>2</sub> and steam-blown process is about of 10–18 MJ/m<sup>3</sup> [56]. Biomass gasification process includes pre-heating, drying, pyrolysis, char gasification, char oxidation and ash formation steps. The obtained cleaned gas can be utilized for heat or electrical power generation [57]. Nowadays many studies have been carried out on biomass gasification indirectly for conversion of it to the combustible gases [58,59]. In order to evaluate the gasification reaction, it is assumed that the energy efficiency is defined as the ratio of the total energy of the desired products to the total input energy [60]. In this case, for achieving to the desired result, the products are considered a mixture of H<sub>2</sub>O, Nitrogen (N<sub>2</sub>), H<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, CO, NH<sub>3</sub> and H<sub>2</sub>S. In this case, char is known as the solid carbon (C) and also tar is not considered in the simulation [6].

### 3.1. Gasification reactions

The gasification reaction arises from chemical reactions between carbon in the char and steam, CO<sub>2</sub> and H<sub>2</sub> in the reactor, as well as chemical reactions between the evolved gases. In principle, gasification process involves the following reactions:

Combustion reactions [57]:

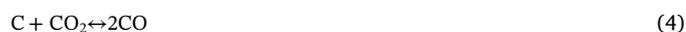


**Table 1**  
Ultimate analysis and LHV of selected biomass feedstock material [53].

Biomass type	Ultimate analysis (db, wt% /wt.)					Proximate analysis (wt% /wt.)				LHV (MJ/kg)
	C	H	O	N	S	ASH	VM	FC	M	
Cedar wood	51.1	5.9	42.5	0.12	0.02	0.3	80–82	18–20	0	19.26
Wood sawdust	46.2	5.1	35.4	1.5	0.06	1.3	70.4	17.9	10.4	18.81
Olive oil residue	50.7	5.89	36.97	1.36	0.3	4.6	76	19.4	9.5	21.2
Rice husk	45.8	6	47.9	0.3	0	0.8	73.8	13.1	12.3	13.36
Rice straw	38.61	4.28	37.16	1.08	0.65	12.64	65.23	16.55	5.58	14.4
Pine sawdust	50.54	7.08	41.11	0.15	0.57	0.55	82.29	17.16	0	20.54
Spruce wood pellet	49.3	5.9	44.4	0.1	0	0.3	74.2	17.1	8.4	18.5
Coffee husk	46.8	4.9	47.1	0.6	0.6	1	74.3	14.3	10.4	16.54
Coffee ground	52.97	6.51	36.62	2.8	0.05	1	71.8	16.7	10.5	22
Larch wood	44.18	6.38	49.32	0.12	0	0.12	76.86	14.86	8.16	19.45
Grapevine pruning waste	46.97	5.8	44.49	0.67	0.01	2.06	78.16	19.78	0	17.91
Jute stick	49.79	6.02	41.37	0.19	0.05	0.62	76–78	21.4–23.4	0	19.66
Sugar-cane bagasse	48.58	5.97	38.94	0.2	0.05	1.26	67–70	28.74–30.74	0	19.05
Corn cob	40.22	4.11	42.56	0.39	0.04	2.97	71.21	16.11	9.71	16.65
Peach stone	51.95	5.76	40.7	0.79	0.01	0.65	81.3	18.1	8.53	21.6
Wheat straw	46.1	5.6	41.7	0.5	0.08	6.1	75.8	18.1	0	17.2
Cotton stem	42.8	5.3	38.5	1	0.2	4.3	72.3	15.5	7.9	15.2
Straw	36.57	4.91	40.7	0.57	0.14	8.61	64.98	17.91	8.5	14.6
Camphor wood	43.43	4.84	38.53	0.32	0.1	0.49	72.47	14.75	12.29	17.48
Beech wood	48.27	6.36	45.2	0.14	0	0.8	81	18	0	19.2
Switchgrass	47	5.3	41.4	0.5	0.1	4.6	58.4	17.1	20	18.7
Oil Palm Shell	53.78	7.2	36.3	0	0.51	2.21	73.74	18.37	50	22.14
Wood Chip	51.19	6.08	41.3	0.2	0.02	1.16	80	18.84	20	19.9



Boudouard reaction [57,61]:



Water-gas reaction [61]:



Methanation reaction [57,61]:



### 3.2. Gasification effective parameters

Significant operating parameters which affect the gasification process are gasifying agent and feedstock flow rates, equivalence ratio, reactor temperature and pressure [62]. Any changing in the effective parameters affect the end-gas composition and performance of the gasifier as well [62]. Also, there is a natural heterogeneity in different feedstocks in terms of composition and thermo-chemical properties [63]. It is also noticed that these parameters have an influence on the gasification process and thus demonstrate an interrelated behavior [56,64] (see Table 2).

## 4. Process simulation

A FORTRAN subroutine with Aspen plus software is demonstrated to control the process yields. In the Aspen plus, process streams include mass or energy flows. The role of Aspen plus is to divide the material streams into three categories: mixed, solid, and non-conventional (for substances like biomass) [65]. Mixed streams are composed of mixtures of components, which can be in three different phases: liquid, gaseous and solid. In this simulation, component of the solid phase is C. From the simulator libraries, thermodynamic properties of the chemical components are defined. Non-conventional components are defined by implementing the standard enthalpy of formation of them. The elementary composition (ultimate and proximate analyses) of the components are also defined. In this case, the biomass composition can be characterized by the simulator.

### 4.1. Assumptions

The utilized assumptions for modeling of the biomass gasification process are as follows:

- The process is in the steady state and isothermal conditions [66].
- The gasification process is carried out without using a catalyst.
- Devolatilization of the biomass takes place immediately and volatile gas products are mostly composed of CO, CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>O.
- Particles have a spherical shape with the uniform size and the

constant average diameter during the gasification, which are all based on the shrinking core model [67].

- All gases have a uniform distribution with emulsion phase.
- All gases and their properties are same as the ideal gases.
- Composition of the air component is 79% N<sub>2</sub> and 21% O<sub>2</sub> [68].
- Tar (C<sub>18</sub>H<sub>12</sub>) is modeled as an aromatic compound [69].

### 4.2. Simulation of the input parameters

This section outlines the input data to the simulator as well as the chosen calculation methods. Additionally, descriptions about the utilized flowsheets are presented in details.

#### 4.2.1. Setup and calculation methods

To have solid state input and output streams, “Solids with metric units” was chosen as the flowsheet type [61]. To setup the flowsheet, MCINPSD stream class should be set to the simulation. With this setup, it is possible aqueous streams (MIXED), conventional solid streams (CIPSD) and non-conventional solid streams (NCPSD) to be considered and analyzed during the simulation. After that, the process type is chosen COMMON because it is assigned as a general industry type which is against simulation of chemical, petrochemical and pharmaceutical. IDEAL base calculation method is chosen, so phase equilibrium calculations are done based on the Raoult's Law, Henry's Law, ideal gas law, etc. [70].

#### 4.2.2. Component definition and inputs

Modeling of the solid biomass is done by using a user-defined, non-conventional solid, based on the ultimate, proximate, and sulfur analyses. In this regard, these parameters are utilized as input for simulation of the biomass gasification. Sulfur analyses are set to zero since the density and enthalpy of the coal are considered as the density and enthalpy of the biomass. DCOALIGHT and HCOALGEN methods are implemented for calculation of the density and enthalpy [71]. Modeling of the fluid streams is done by the conventional components which their thermos-physical data has been saved in the ASPEN Plus databanks. Under consideration components are CO, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>, H<sub>2</sub>O and O<sub>2</sub>.

### 4.3. Utilized stages of the simulation

Drying and decomposition of the feed, volatile reactions and gas-solid separation are the used simulation stages of the overall gasification process [72].

#### 4.3.1. Drying

Typically, the biomass moisture is about 5–50%. Removing of this moisture is done in the drying step. For simulation of this part, a yield reactor (Rstoic) is used. Drying occurs at the temperature about of 80–200 °C to decrease the moisture of the feed to a value less than 10% [73].

#### 4.3.2. Biomass decomposition

In this step, biomass is converted into the C, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, S and ash by determining the distribution according to the biomass ultimate analysis [74]. Simulation of the feed decomposition is done by yield reactor

**Table 2**  
The steam gasification parameters effects on H<sub>2</sub> yield [55].

Parameter	Description	Effects
Biomass types	Different plant species wastes	Product composition largely depends of inherent nature of parent biomass.
Process temperature	Gasifier temperature is considered after pyrolysis zone	Low temperatures favours char yield and CH <sub>4</sub> production. Optimal temperatures for H <sub>2</sub> generation 800–900 °C.
Steam-biomass ratio	Mass of steam/mass of biomass	Low S/B e CH <sub>4</sub> and char, High S/B e syngas.
Process pressure	Gasification occurs at constant pressure	The chemical equilibrium indicates that gasification is favoured by low pressures and high temperatures. However, no substantial gain is obtained if the process runs in vacuum.

(RYIELD).

### 4.3.3. Volatile separation

In this step, a column model is used to separate the solids from the volatile materials [3]. After separation, the next step would be combustion of the volatile components which is done by Gibbs reactor, RGIBBS, with the assumption that reaction follows Gibbs equilibrium. The main components of the biomass are C, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, ash, sulfur, chlorine and moisture. The C which forms a part of the gas phase participates in devolatilization process. Remaining of the C from the biomass which is in the solid phase (char), participates in the char gasification. With the assumption that C and ash are the sole components of the char, amount of C in the gas phase can be calculated by deduction of char carbon from the biomass carbon. Table 3 presents description of the reactor blocks.

### 4.4. Process description

In the gasification process, heating and drying steps are endothermic and consequently, a heat source is necessary. In this regard, the required heat duty can be supplied via indirect heating from an external source as a utility. Approximately 25% excess air or O<sub>2</sub> is required to have complete combustion of the fuel. During the combustion, sufficient heat is released that can be used for drying, pyrolysis and the subsequent endothermic chemical reactions [75]. The main focus of this research is on the gasification process. R-GIBBS block reactor is used for the simulation. This kind of the block is suitable for reactions with known temperature and pressure and unknown reactions stoichiometry. Single-phase chemical equilibrium, or simultaneous phase and chemical equilibrium, by minimizing the Gibbs free energy, based on the atom balance are the assumptions considered through simulation of this reactor. In this study Rice husk, Larch wood and Wood Chip as feedstocks are chosen for the analysis. Table 4 shows comparison of the chosen feedstocks. The plant capacity is arranged to be 10–32 kg/s.

Biomass at 298 K and 1 atm is mixed with the produced solids in the process, 9, and enters the Dry reactor. In this reactor, additional biomass moisture is evaporated via hot air (363 K, 1 atm). For separation of the produced hot gases in the Dry reactor, 1, follows to the Dry flash. In this separator, vapor phase is separated from the solid and leave the reactor as stream 3. After drying, the biomass gasification is performed. Generally, gasification is done based on the indirect heating in low temperature which consists of one decomposition reactor and two combustion reactors. Dry biomass, 2, enters the decomposition reactor. Decomposition is done based on the RYield reactor at 394 K and 1 atm. In this reactor, the biomass is converted to C, O<sub>2</sub>, H<sub>2</sub>, sulfur (S), N<sub>2</sub> and Ash. Outlet stream, 4, and steam at 900 K and 1 atm for production of synthesis gas enter the gasifier. An R-Gibbs reactor model at 900 K and 1 atm is used for simulation of this reactor. For separation of the produced synthesis gas, the outlet stream, 5, follows to the Cyclone 1. The remained solid stream, 7, is Tar (C<sub>18</sub>H<sub>12</sub>). Tar and steam at 723 K and 1 atm enter the second combustion reactor and C and synthesis gas are produced. For separation of the C, stream 8 follows to the second cyclone. After separation, the remained C, 9, is returned to the process and is mixed with fresh biomass. The outlet synthesis gas, 6, is at high temperature so it can be used for production of the stream and air

**Table 3**  
The reactor blocks description in the simulation [3].

Reactor block	Description
RSTOIC	Indicates the stoichiometric model of the reactor with specified reaction extent or conversion. Reactors where reaction kinetics are unknown but stoichiometry and extent of reaction are known.
RYIELD	Indicates the models of the reactor by specifying reaction yields of each process component. This model is useful when reaction stoichiometry and kinetics are unknown and yield distribution data or correlations are available.
RGIBBS	Indicates the single-phase chemical equilibrium, or simultaneous phase and chemical equilibrium by minimizing Gibbs free energy, subject to atom balance constraints. This model is useful when temperature and pressure are known, but the reaction stoichiometry is unknown.

**Table 4**  
Proximate and ultimate analyses and other data for Rice husk, Larch wood and Wood chip [53,76].

Type biomass	Rice husk	Larch wood	Wood Chip
Proximate analysis (wt% dry basis)			
Volatile matter	73.8	76.86	80
Fixed carbon	13.1	14.86	18.84
Ash	0.8	0.12	1.16
Ultimate analysis (wt% dry basis)			
C	45.8	44.18	51.19
H	6	6.38	6.08
O	47.9	49.32	41.3
N	0.3	0.12	0.2
S	0	0	0.02
Moisture content (wt%)	12.3	8.16	20
Lower heating value (MJ/kg)	13.36	19.45	19.09

heating. The produced synthesis gas streams are mixed in Mixer 1. Fig. 1 illustrates the process flow diagram. Also, Tables 5–7 show the thermodynamic data and mass flow rate for the process streams.

## 5. Sensitivity analysis

In this section, effective parameters are chosen to investigate their effect on the gasification process performance. The process outputs based on the different operating conditions are calculated and analyzed.

### 5.1. Hydrogen production yield

Two different analyses, with different steam flow rates (3 kg/s and 7 kg/s) at 900 K is done. The temperature is varied from 80 to 500 K. Biomass flow rate is changed from 10 kg/s to 32 kg/s. Parametric analysis of the steam gasification stage is done in two different modes.

At first, biomass flow rate is changed at fixed steam flow rate gasifier temperature. Next, gasifier temperature is changed at constant amount of steam and biomass.

### 5.2. Type of the biomass

Table 8 presents results of the analysis for various types of the biomasses. Efficiency of the gasifier for production of syngas is defined as the rate of chemical energy of the generated gas over the energy content of the biomass feed as follows [63,77]:

$$\eta_{cg} = \frac{\dot{m}_{prodg} LHV_{prodg}}{\dot{m}_{drybio} LHV_{drybio} + \dot{m}_{steam} LHV_{steam}} \quad (8)$$

Additionally, energy efficiency of hydrogen production in a gasification process can be calculated as follows:

$$\eta_{H_2} = \frac{\dot{m}_{H_2} LHV_{H_2}}{\dot{m}_{drybio} LHV_{drybio} + \dot{m}_{steam} LHV_{steam}} \quad (9)$$

Table 8 presents the gasification efficiency for different types of the biomass.  $\eta_{cg}$  for Wood Chip, Spruce wood pellet, Peach stone, Pine sawdust and Rice husk is higher than 95%. Also,  $\eta_{H_2}$  for these biomasses is about 50%.

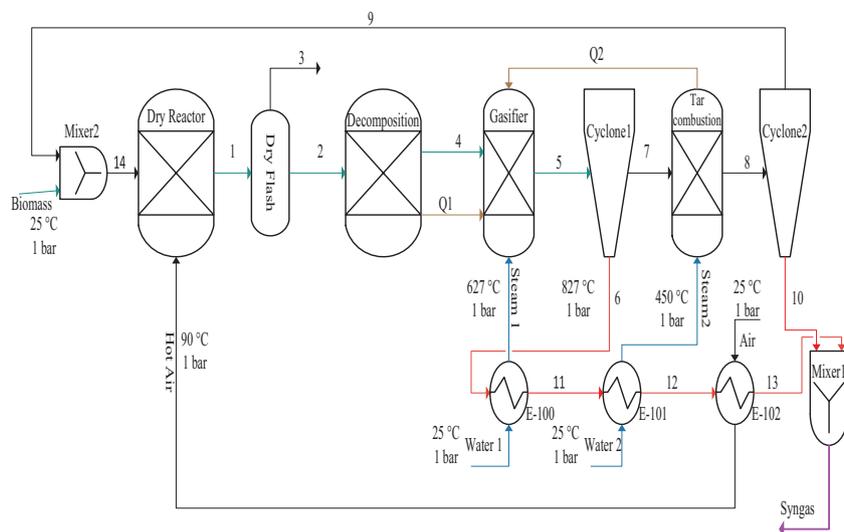


Fig. 1. The flow diagram of the process.

Table 5

The specifications of the process stream for the Rice husk.

	Biomass	Air	Hot Air	Water1	Steam1	Water2	Steam2	Syngas	1	2	3
Temperature (°C)	25	25	90	25	627	25	450	209	41	41	41
Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1
Mass Flow (kg/h)	72000	108000	108000	16200	16200	14400	14400	100760	182125	72285	109840
Mass Enthalpy (KW)	24907	- 8	1970	- 71873	- 54927	- 63887	- 50352	- 104490	27192	33569	- 6377
Mass flow rate (kg/h)											
H <sub>2</sub> O	0	0	0	16200	16200	14400	14400	8381	1840	0	1840
N <sub>2</sub>	0	82845	82845	0	0	0	0	195	82845	0	82845
O <sub>2</sub>	0	25155	25155	0	0	0	0	20487	25155	0	25155
CO <sub>2</sub>	0	0	0	0	0	0	0	8197	0	0	0
SO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
H <sub>2</sub>	0	0	0	0	0	0	0	6439	0	0	0
CO	0	0	0	0	0	0	0	54039	0	0	0
H <sub>2</sub> S	0	0	0	0	0	0	0	0	0	0	0
NH <sub>3</sub>	0	0	0	0	0	0	0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
CH <sub>4</sub>	0	0	0	0	0	0	0	3021	0	0	0
C	0	0	0	0	0	0	0	0	2125	2125	0
S	0	0	0	0	0	0	0	0	0	0	0
Tar	0	0	0	0	0	0	0	0	0	0	0
Biomass	72000	0	0	0	0	0	0	0	70160	70160	0

	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	1251	827	827	827	449	449	449	482	195	152	34
Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1
Mass Flow (kg/h)	72285	88485	81392	7093	21493	2125	19368	81392	81392	81392	74125
Mass Enthalpy (KW)	33916	- 21056	- 23873	2817	- 47837	322	- 48159	- 40819	- 54355	- 56334	25222
Mass flow rate (kg/h)											
H <sub>2</sub> O	7228	782	782	0	7599	0	7599	782	782	782	0
N <sub>2</sub>	195	195	195	0	0	0	0	195	195	195	0
O <sub>2</sub>	31162	20487	20487	0	0	0	0	20487	20487	20487	0
CO <sub>2</sub>	0	121	121	0	8076	0	8076	121	121	121	0
SO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
H <sub>2</sub>	3903	6062	6062	0	378	0	378	6062	6062	6062	0
CO	0	53744	53744	0	295	0	295	53744	53744	53744	0
H <sub>2</sub> S	0	0	0	0	0	0	0	0	0	0	0
NH <sub>3</sub>	0	0	0	0	0	0	0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
CH <sub>4</sub>	0	0	0	0	3021	0	3021	0	0	0	0
C	29796	0	0	0	2125	2125	0	0	0	0	2125
S	0	0	0	0	0	0	0	0	0	0	0
Tar	0	7093	0	7093	0	0	0	0	0	0	0
Biomass	0	0	0	0	0	0	0	0	0	0	72000

**Table 6**  
The specifications of the process stream for the Larch wood.

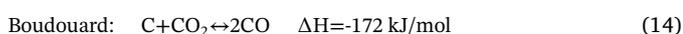
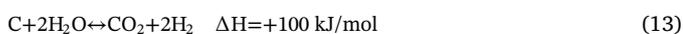
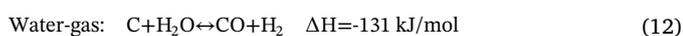
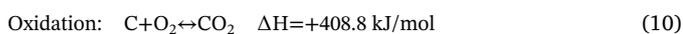
	Biomass	Air	Hot Air	Water1	Steam1	Water2	Steam2	Syngas	1	2	3
Temperature (°C)	25	25	90	25	627	25	450	234	162	162	162
Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1
Mass Flow (kg/h)	72000	108000	108000	16200	16200	14400	14400	102600	183846	75846	108000
Mass Enthalpy (KW)	40842	– 8	1970	– 71873	– 54927	– 63887	– 50352	– 99107	43417	39252	4164
Mass flow rate (kg/h)											
H <sub>2</sub> O	0	0	0	16200	16200	14400	14400	8390	0	0	0
N <sub>2</sub>	0	82845	82845	0	0	0	0	82	82845	0	82845
O <sub>2</sub>	0	25155	25155	0	0	0	0	25197	25155	0	25155
CO <sub>2</sub>	0	0	0	0	0	0	0	8185	0	0	0
SO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
H <sub>2</sub>	0	0	0	0	0	0	0	6909	0	0	0
CO	0	0	0	0	0	0	0	50734	0	0	0
H <sub>2</sub> S	0	0	0	0	0	0	0	0	0	0	0
NH <sub>3</sub>	0	0	0	0	0	0	0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
CH <sub>4</sub>	0	0	0	0	0	0	0	3103	0	0	0
C	0	0	0	0	0	0	0	0	3846	3846	0
S	0	0	0	0	0	0	0	0	0	0	0
Tar	0	0	0	0	0	0	0	0	0	0	0
Biomass	72000	0	0	0	0	0	0	0	72000	72000	0

	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	1298	827	827	827	468	468	468	495	219	178	41
Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1
Mass Flow (kg/h)	75846	92046	83012	9034	23434	3846	19588	83012	83012	83012	75846
Mass Enthalpy (KW)	39600	– 15372	– 18960	3588	– 47066	620	– 47686	– 35907	– 49442	– 51421	41447
Mass flow rate (kg/h)											
H <sub>2</sub> O	7585	871	871	0	7519	0	7519	871	871	871	0
N <sub>2</sub>	82	82	82	0	0	0	0	82	82	82	0
O <sub>2</sub>	33666	25197	25197	0	0	0	0	25197	25197	25197	0
CO <sub>2</sub>	0	119	119	0	8066	0	8066	119	119	119	0
SO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
H <sub>2</sub>	4355	6440	6440	0	469	0	469	6440	6440	6440	0
CO	0	50303	50303	0	432	0	432	50303	50303	50303	0
H <sub>2</sub> S	0	0	0	0	0	0	0	0	0	0	0
NH <sub>3</sub>	0	0	0	0	0	0	0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
CH <sub>4</sub>	0	0	0	0	3103	0	3103	0	0	0	0
C	30158	0	0	0	3846	3846	0	0	0	0	3846
S	0	0	0	0	0	0	0	0	0	0	0
Tar	0	9034	0	9034	0	0	0	0	0	0	0
Biomass	0	0	0	0	0	0	0	0	0	0	72000

### 5.3. Gasification temperature

One of the main operating parameters of the gasification process is bed temperature which can affect the heating value and composition of the produced syngas [78]. This temperature based on the Le' Chatlier's principle can affect the gasification reactions and consequently the produced gas compositions. In endothermic reactions, formation of the product increases with temperature. The main reactions in the gasification process are illustrated as follows [53,79,80]:



The main objective of the gasification process is producing a combustible gas mixture which is rich in CO, H<sub>2</sub> and CH<sub>4</sub> with medium to high rate of LHV which is appropriate for further operation in turbines and internal combustion engines [81]. What is clear is that, with increasing the gasification temperature, heating value of the produced gas decreases. The required heat for gasification is supplied by combustion enthalpy of the biomass, so increasing the temperature improves biomass combustion which consequently results in more CO<sub>2</sub> and N<sub>2</sub> and

lowers heating value [82]. Besides, increase in bed temperature enhances C conversion and reforming of tars and steam cracking, that lead to less char and consequently tar formation and high gas production [83]. Figs. 2 to 4 illustrate outlet gas concentration versus gasification temperature for Rice husk, Larch wood and Wood chip respectively. Biomasses and steam's mass flow rates are 20 kg/s and 4.5 kg/s respectively. H<sub>2</sub> generation increases with temperature. Over the studied temperatures, some changes in the gas yield are observed. Gasification temperature can affect the H<sub>2</sub> production significantly in all cases.

### 5.4. Effect of biomass quantity on hydrogen production

Figs. 5–7 show effect of the biomass flow rate on the outlet gas composition with the assumption that other parameters are constant; steam rate is 4.5 kg/s and the gasifier's temperature is 1100 K. H<sub>2</sub> concentration almost increases from 48% to 56%. CH<sub>4</sub> concentration varies by different amounts of biomass.

Figs. 8–10 illustrate produced H<sub>2</sub> and gasification ratio versus the biomass flow rate. In all cases, H<sub>2</sub> fraction decreases with the biomass flow rate. However, H<sub>2</sub> flow rate increases with the biomass flow rate.

### 5.5. Effect of supplied steam

Figs. 11–13 show concentration of the outlet gases against the steam flow rate when the biomass flow rate and gasifier temperature are fixed

**Table 7**  
The specifications of the process stream for the Wood chip.

	Biomass	Air	Hot Air	Water1	Steam1	Water2	Steam2	Syngas	1	2	3
Temperature (°C)	25	25	90	25	627	25	450	169	50	50	50
Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1
Mass Flow (kg/h)	72000	108000	108000	16200	16200	14400	14400	94600	180000	64000	116000
Mass Enthalpy (KW)	- 41343	- 8	1970	- 71873	- 54927	- 63887	- 50352	- 142960	- 34203	- 5224	- 28979
Mass flow rate (kg/h)											
H <sub>2</sub> O	0	0	0	16200	16200	14400	14400	16064	8000	0	8000
N <sub>2</sub>	0	82845	82845	0	0	0	0	115	82845	0	82845
O <sub>2</sub>	0	25155	25155	0	0	0	0	0	25155	0	25155
CO <sub>2</sub>	0	0	0	0	0	0	0	7776	0	0	0
SO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
H <sub>2</sub>	0	0	0	0	0	0	0	5691	0	0	0
CO	0	0	0	0	0	0	0	64325	0	0	0
H <sub>2</sub> S	0	0	0	0	0	0	0	12	0	0	0
NH <sub>3</sub>	0	0	0	0	0	0	0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0	0	0	0	0	0	0
CH <sub>4</sub>	0	0	0	0	0	0	0	617	0	0	0
C	0	0	0	0	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0
Tar	0	0	0	0	0	0	0	0	0	0	0
Biomass	72000	0	0	0	0	0	0	0	64000	64000	0

	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	549	827	827	827	364		364	473	176	132	25
Pressure (atm)	1	1	1	1	1		1	1	1	1	1
Mass Flow (kg/h)	64000	80200	79035	1165	15565	0	15565	79035	79035	79035	72000
Mass Enthalpy (KW)	- 4877	- 59849	- 60311	463	- 50192	0	- 50192	- 77258	- 90793	- 92772	- 41340
Mass flow rate (kg/h)											
H <sub>2</sub> O	6403	3680	3680	0	12384		12384	3680	3680	3680	0
N <sub>2</sub>	115	115	115	0	0		0	115	115	115	0
O <sub>2</sub>	23800	0	0	0	0		0	0	0	0	0
CO <sub>2</sub>	0	5320	5320	0	2456		2456	5320	5320	5320	0
SO <sub>2</sub>	0	0	0	0	0		0	0	0	0	0
H <sub>2</sub>	3504	5548	5548	0	143		143	5548	5548	5548	0
CO	0	64316	64316	0	9		9	64316	64316	64316	0
H <sub>2</sub> S	0	12	12	0	0		0	12	12	12	0
NH <sub>3</sub>	0	0	0	0	0		0	0	0	0	0
NO <sub>2</sub>	0	0	0	0	0		0	0	0	0	0
CH <sub>4</sub>	0	44	44	0	573		573	44	44	44	0
C	30167	0	0	0	0		0	0	0	0	0
S	12	0	0	0	0		0	0	0	0	0
Tar	0	1165	0	1165	0		0	0	0	0	0
Biomass	0	0	0	0	0		0	0	0	0	72000

**Table 8**  
The gasification efficiency for different types of biomasses.

Type Biomass	$\eta_{cg}$	H <sub>2</sub> /syngas	$\eta_{H_2}$
Cedar wood	0.92	0.58	0.50
Wood sawdust	0.69	0.69	0.45
Olive oil residue	0.96	0.57	0.50
Rice husk	0.98	0.62	0.57
Rice straw	0.50	0.98	0.49
Pine sawdust	0.97	0.57	0.52
Spruce wood pellet	0.94	0.56	0.49
Coffee husk	0.72	0.68	0.46

at 20 kg/s and 1100 K, respectively. The results show that H<sub>2</sub> mol% decreases from 54% to 51.2% for Rice husk, 55.5–53.3% for Larch wood and 51.8–50.2% for Wood chip (Fig. 14).

## 6. Energy and exergy analyses

### 6.1. Energy analysis

Energy conservation which is known as the first law of thermodynamics for a control volume is described as follows [6,57,84]:

$$\sum_i \dot{E}_i = \sum_e \dot{E}_e \tag{16}$$

$$\sum_{i=1}^N \dot{m}_i h_i + \dot{Q}_{net} = \sum_{j=1}^M \dot{m}_j h_j + \dot{W}_{net} \tag{17}$$

$\dot{Q}_{net}$  and  $\dot{W}_{net}$  represent the net heat and power rate over the component boundaries. Gasification is an endothermic process without any kinds of the work. The required heat energy of the process is provided by itself and heat loss from the gasifier wall is used for heating. Gasification process is similar to the other processes and it must satisfy the first law of thermodynamics as follows:

$$\sum_R H_i - \sum_P H_j = \dot{Q}_{lostwa} \tag{18}$$

$\dot{Q}_{lostwa}$  is the energy loss during the process and  $H$  is the products and reactants enthalpy and can be calculated as follows:

$$H_i = \dot{m}_i h_i \tag{19}$$

$$H_j = \dot{m}_j h_j \tag{20}$$

Subscripts  $i$  and  $j$  are used to declare reactants and products, respectively. Letters  $R$  and  $P$  are used to show the number of reactants and products. Ideal gas rule is used for the gases, so their enthalpies and entropies can be calculated as follows:

$$h = h_f^o + \Delta h \tag{21}$$

$$\Delta h = \int_{T_0}^T C_p dT \tag{22}$$

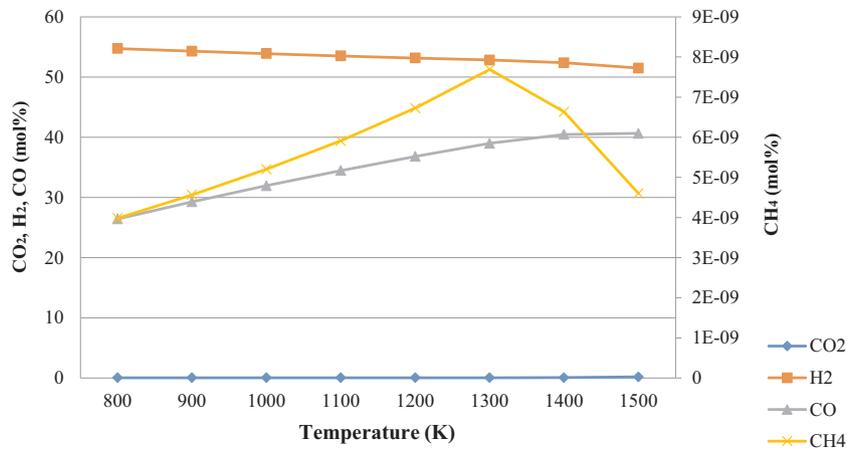


Fig. 2. Outlet gas concentration versus gasification temperature for Rice husk (20 kg/s) and steam (4.5 kg/s).

$$\Delta s = \int_{T_0}^T \frac{C_p}{T} dT \quad (23)$$

The term  $C_p$  which is specific heat at constant pressure for the gases at the gasifier's temperature can be calculated by Eq. (24):

$$C_p = a' + b'T + c'T^2 + d'T^3 \quad (24)$$

Table 9 shows the coefficients,  $a'$ ,  $b'$ ,  $c'$  and  $d'$  for the used gases. Specific heat of tar in coal gasification is based on the presented methods by Hyman et al. [69] as follows:

$$C_p = 0.00422T \text{ (kJ/kgtar. K)} \quad (25)$$

Eqs. (26) and (27) are used for calculation of the enthalpy and the entropy of tar [85]. The term which is related to the sulfur is not considered because the used biomasses have a small percentage of it:

$$h_{tar} = h_{tar}^o + \int_{T_0}^T C_p dT \quad (26)$$

$$h_{tar}^o = -30.980 + X_{CO_2} h_{CO_2}^o + X_{HO_2} h_{HO_2}^o \quad (27)$$

$X_i$  is mole fraction and  $h_i^o$  is the standard enthalpy of formation for species  $i$ . Entropy of the tar is calculated as follows:

$$s = s_{tar}^o + \int_{T_0}^T \frac{C_p}{T} dT \quad (28)$$

The standard tar entropy,  $s_{tar}^o$  in kJ/kmol-K is calculated as follows:

$$s_{tar}^o = a_1 + a_2 \exp \left[ -a_3 \left( \frac{H}{C} + N \right) \right] + a_4 \left( \frac{O}{C+N} \right) + a_5 \left( \frac{N}{C+N} \right) + a_6 \left( \frac{S}{C+N} \right) \quad (29)$$

where  $a_1 = 37.1635$ ,  $a_2 = -31.4767$ ,  $a_3 = 0.564682$ ,  $a_4 = 20.1145$ ,  $a_5 = 54.3111$  and  $a_6 = 44.6712$ . Also, C, H, N, O and S are C, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub> and sulfur are weight fractions of this components in the used biomass.

Losses from the gasifier to the environment in comparison with the energy entering or leaving is negligible [57,87]. However, for reaching to more accurate results, these losses are considered in this study. Energy loss related to the heat transfer to the environment  $\dot{Q}_{lostwa}$  is calculated as follows:

$$\dot{Q}_{lostwa} = U_{wa} A (T_w - T_o) \quad (30)$$

The overall heat transfer coefficient,  $U_{wa}$  between the gasifier external wall at a temperature of ( $T_w$ ) and the ambient temperature ( $T_o$ ) is calculated by the Eq. (31) [88]:

$$U_{wa} = 1.9468(T_w - T_o)^{1/4} (2.8633U_o + 1)^{1/2} + 5.75 \times 10^{-8} \epsilon_{ins} \frac{T_w^4 - T_o^4}{T_w - T_o} \quad (31)$$

$U_o$  is the average velocity of the wind and it is supposed to be 2 m/s.  $T_w$  is calculated from the energy balance around the gasifier's wall. It is considered that wall is insulated with a material with  $x_{ins}$  thickness and thermal conductivity of  $k_{ins}$  by Eq. (32):

$$U_{wa} (T_w - T_o) = \frac{k_{ins}}{x_{ins}} (T - T_w) \quad (32)$$

### 6.1.1. Energy efficiency of the gasifier

The gasified biomass energy flow,  $En_{Biomass}$ , is calculated by multiplying its lower heating value to its mass flow rate,  $\dot{m}_{Biomass}$  as follows:

$$En_{Biomass} = \dot{m}_{Biomass} LHV_{Biomass} \quad (33)$$

Three forms of energetic efficiencies,  $\eta_{en1}$ ,  $\eta_{en2}$  and  $\eta_{en3}$  are defined as follows:

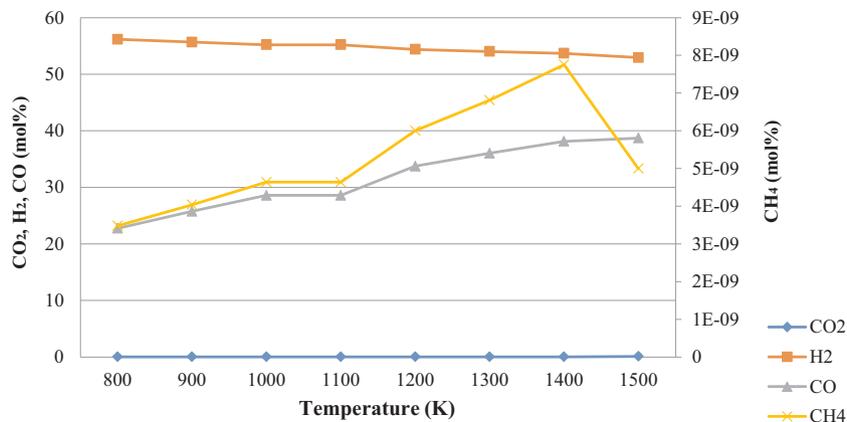


Fig. 3. Outlet gas concentration versus gasification temperature for Larch Wood (20 kg/s) and steam (4.5 kg/s).

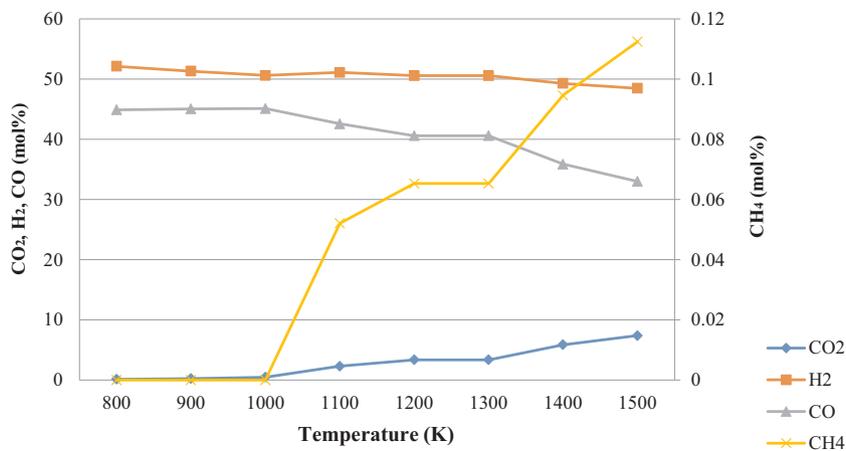


Fig. 4. Outlet gas concentration versus gasification temperature for Wood chip (20 kg/s) and steam (4.5 kg/s).

$$\eta_{en1} = \frac{En_{H_2}}{En_{Biomass} + En_{steam}} \quad (34)$$

$$\eta_{en2} = \frac{En_{gas}}{En_{Biomass} + En_{steam}} \quad (35)$$

$$\eta_{en3} = \frac{En_{gas} + En_{tar}}{En_{Biomass} + En_{steam}} \quad (36)$$

where  $En_{H_2}$ ,  $En_{gas}$ ,  $En_{biomass}$ ,  $En_{tar}$  and  $En_{steam}$  are energy content of the generated  $H_2$ , outlet gases, biomass, tar and injected steam, respectively.

6.2. Exergy analysis

Exergy of a system is the maximum attainable work during a process that brings the system into equilibrium with the environment [89]. Exergy rate is calculated by the following equation [57]:

$$\dot{Ex}_i = \dot{m}_i Ex_i \quad (37)$$

Subscript  $i$  represents the material streams and  $Ex$  shows the specific exergy. The specific exergy is divided into two parts: chemical and physical exergies. Chemical exergy ( $Ex_{ch}$ ) is a function of the material stream composition and can be calculated as follows [90]:

$$Ex_{ch} = \sum_i (X_i Ex_{o,i}) + RT_0 \sum_i (X_i \ln X_i) \quad (38)$$

$X_i$  and  $Ex_{o,i}$  are mole fraction and standard chemical exergy of component  $i$ . Table 10 represents the standard chemical exergy of the

biomass components. The Eq. (38) can be rewritten as follows [91]:

$$Ex_{ch} = \sum_i (X_i Ex_{o,i}) + G - \sum_i (X_i G_i) \quad (39)$$

Where  $G$  and  $G_i$  are Gibbs free energy of the mixture and pure components at environment pressure and temperature of  $P_0$  and  $T_0$ , respectively. In this study, exergy of the biomass is computed by Szargut et al. [92,93] method, which is shown as follows:

$$Ex_{biomass} = \beta LHV_{biomass} \quad (40)$$

Coefficient  $\beta$  is given in terms of  $O_2$ -C and  $H_2$ -C ratios and can be calculated by Eq. (41):

$$\beta = \frac{1.0414 + 0.0177[H/C] - 0.3328[O/C][1 + 0.0537[H/C]]}{1 - 0.4021[O/C]} \quad (41)$$

Another part of exergy, physical exergy ( $Ex_{ph}$ ), depends on the temperature and pressure and is calculated as follows [91]:

$$Ex_{ph} = (h - h_o) - T_o(s - s_o) \quad (42)$$

where  $h$  and  $s$  are the specific enthalpy and entropy, respectively. Also  $h_o$  and  $s_o$  are specific enthalpy and entropy at standard state ( $T_o = 289$  K and  $P_o = 1$  atm), respectively. So, the total exergy ( $Ex$ ) can be calculated by Eq. (43) [94]:

$$Ex = Ex_{ch} + Ex_{ph} \quad (43)$$

The entropy balance is illustrated by the Eq. (44):

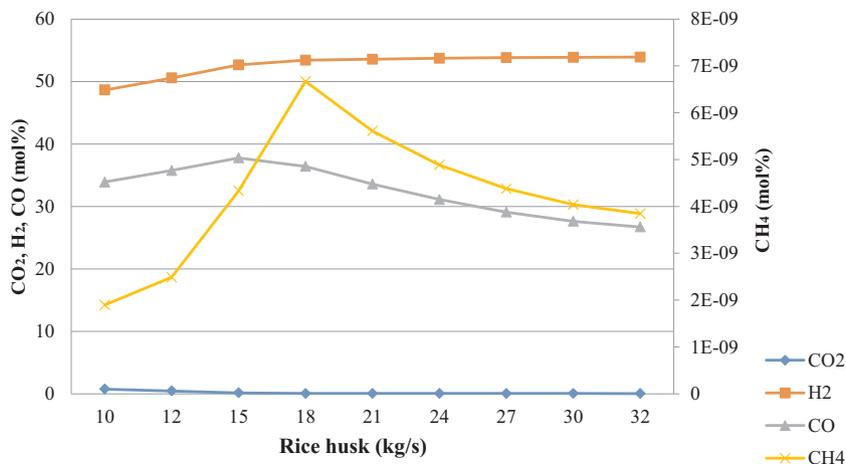


Fig. 5. Outlet gas composition versus Rice husk flow rate (steam rate: 4.5 kg/s and gasifier temperature: 1100 K).

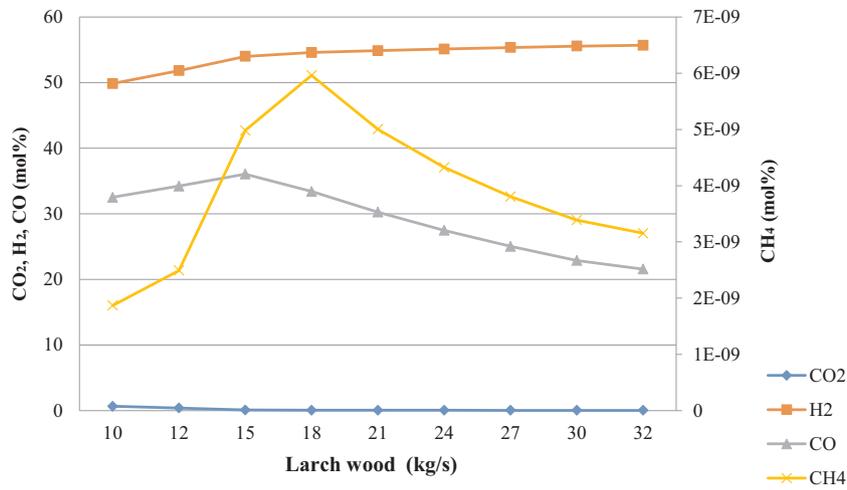


Fig. 6. Outlet gas composition versus Larch Wood flow rate (steam rate: 4.5 kg/s and gasifier temperature: 1100 K).

$$\sum_i \dot{S}_i + \dot{S}_{gen} = \sum_e \dot{S}_e + \Delta \dot{S}_{CV} \tag{44}$$

$\Delta \dot{S}_{CV}$  is the entropy difference due to the heat transfer across the system boundaries. Eq. (44) can be summarized as follows:

$$\sum_i \dot{S}_i + \dot{S}_{gen} = \sum_e \dot{S}_e + \frac{\dot{Q}_{lostwa}}{T_w} \tag{45}$$

Entropy rate ( $\dot{S}$ ) is obtained by multiplying the specific entropy ( $s$ ) and mass flow rate ( $\dot{m}$ ) for the inlet and outlet streams as follows:

$$\dot{S}_i = \dot{m}_i s_i \tag{46}$$

$$\dot{S}_e = \dot{m}_e s_e \tag{47}$$

Heat transfer exergy rate can be obtained by Eq. (48) [95]:

$$\dot{E}x_Q = \dot{Q}_{lostwa} \times (1 - T_0/T_w) \tag{48}$$

### 6.3. Irreversibility rate

For any kinds of the process, from the thermodynamics point of view, must satisfy both first and second laws of thermodynamics. Irreversibility rate is divided into two parts: internal irreversibility and external irreversibility. Internal irreversibility illustrates the internal exergy loss as the quality of material and energy loss due to dissipation. It can be computed in terms of the generated entropy during the gasification process as a consequence of the flow rate of substances, heat

and mass transfer and chemical reactions. It is calculated by the following equation:

$$\dot{E}x_{destin} = T_0 \dot{S}_{gen} \tag{49}$$

Exergy loss from the gasifier wall is calculated as follows:

$$\dot{E}x_{destwa} = \dot{Q}_{lostwa} \left( 1 - \frac{T_0}{T_w} \right) \tag{50}$$

Total exergy destruction rate is calculated as follows [98]:

$$\dot{E}x_{des} = \dot{E}x_{destin} + \dot{E}x_{destwa} \tag{51}$$

Table 11 illustrates exergy of the process material streams. Chemical exergy of the pure components can be calculated by the method represented in [90]. Table 12 shows the used definitions for calculation of the exergy efficiency of the process components. Also, Table 13 presents results of the exergy analysis.

Heat exchanger (E-101) in all cases has the lowest exergy efficiency, while heat exchanger (E-100) has the greatest exergy destruction rate. The lowest exergy destruction rate among the process components is related to the heat exchanger (E-102). Exergy efficiency of the dry Reactor is high (about 90%) in all cases. Nonetheless, exergy destruction rate for this component is a great value against the other process components. For Rice husk type of the biomass, the greatest exergy destruction rate in the process is related to the Tar combustion and decomposition reactors, respectively.

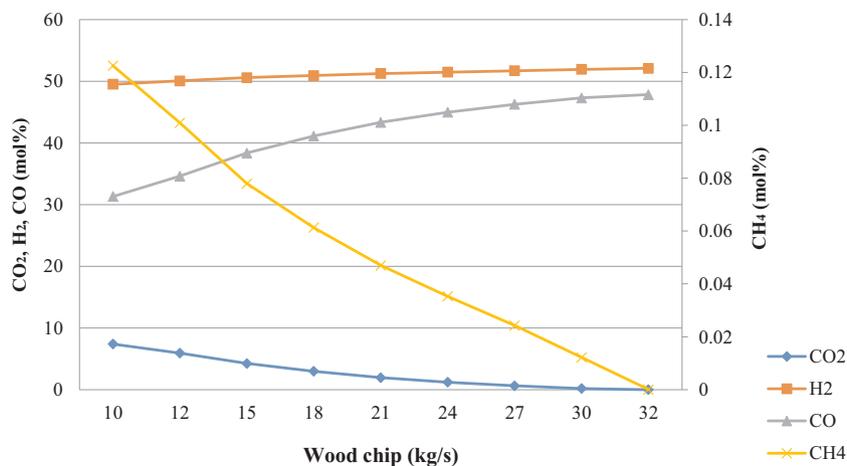


Fig. 7. Outlet gas composition versus Wood chip flow rate (steam rate: 4.5 kg/s and gasifier temperature: 1100 K).

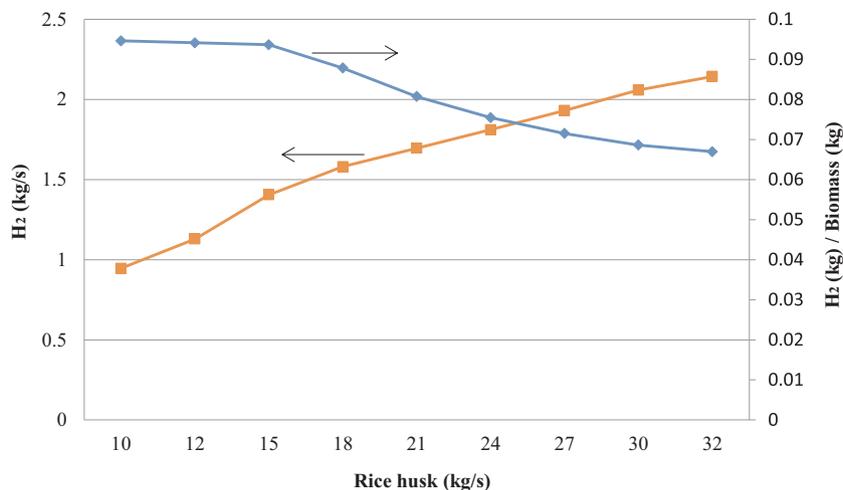


Fig. 8. Produced H<sub>2</sub> and gasification ratio versus biomass flow rate (Rice husk).

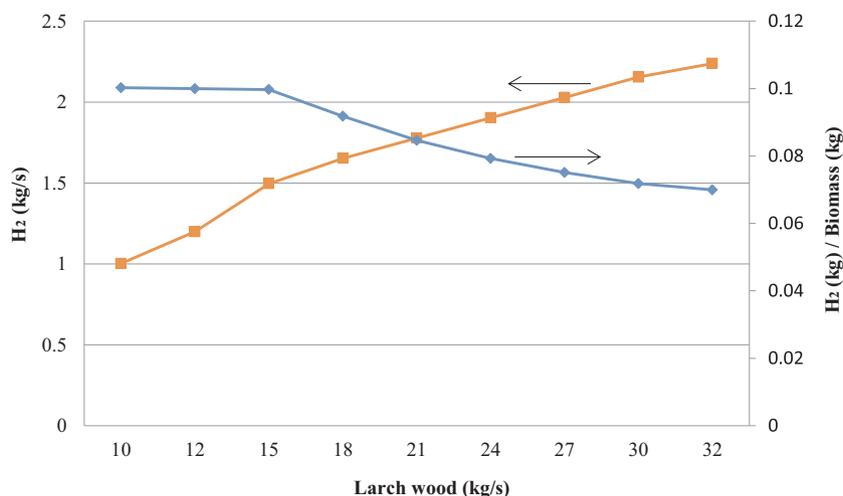


Fig. 9. Produced H<sub>2</sub> and gasification ratio versus biomass flow rate (Larch Wood).

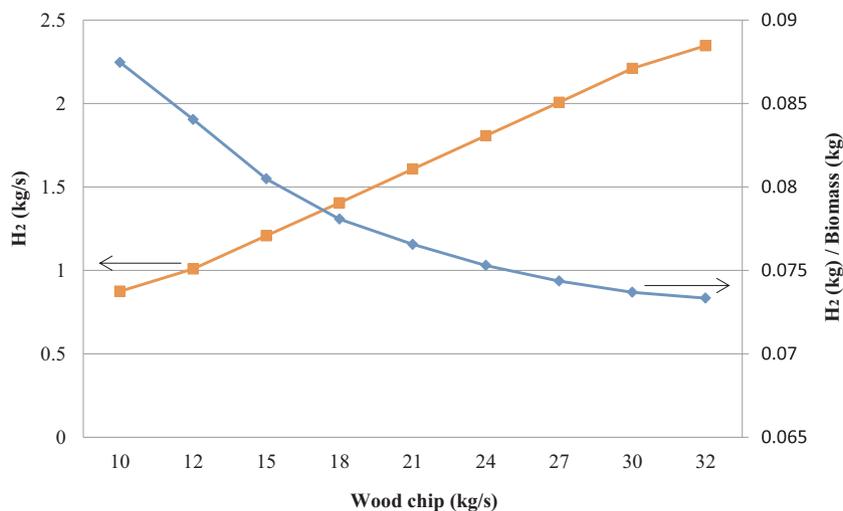


Fig. 10. Produced H<sub>2</sub> and gasification ratio versus biomass flow rate (Wood chip).

7. Hydrogen production from the biomass gasification

For further analyses of the biomass gasification process, hydrogen production via this process is developed and discussed in details. H<sub>2</sub>

production from the biomass can be done by utilizing water-gas shift reaction (WGSR). This process mainly includes six parts [100]. Biomass drying, biomass decomposition and gasification by the reactors, compression and purifying of the produced syngas, steam methane

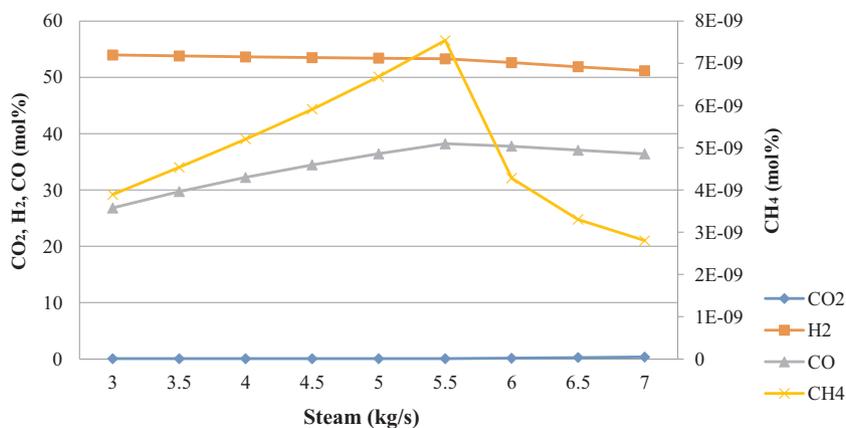


Fig. 11. The concentration of the outlet gases against steam flow rate (Rice husk at 1100 K).

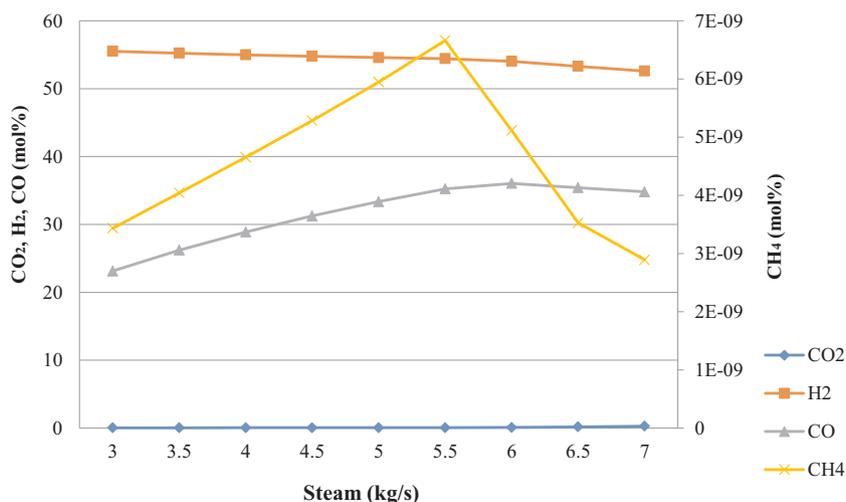


Fig. 12. The concentration of the outlet gases against steam flow rate (Larch wood at 1100 K).

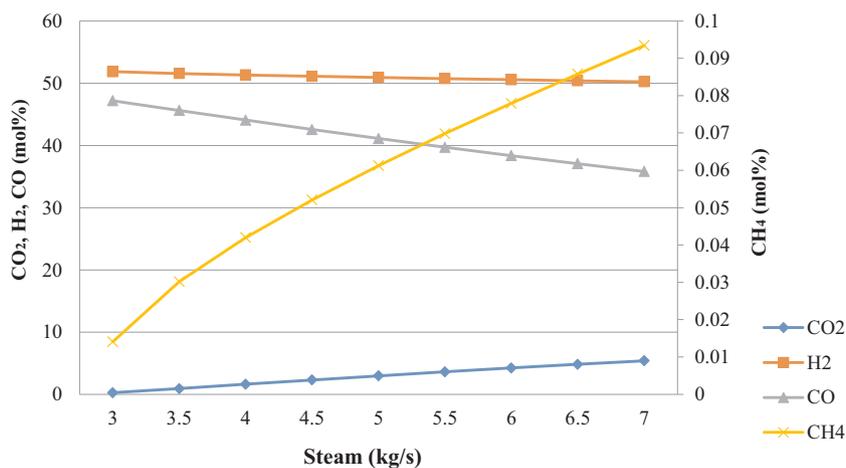


Fig. 13. The concentration of the outlet gases against steam flow rate (Wood chip at 1100 K).

reforming (SMR), WGS reactions at a high and low temperature (HTS and LTS) and finally separation of H<sub>2</sub> from CO<sub>2</sub> by using pressure swing adsorption (PSA) unit. Drying step consists of the reactor and two-phase separator. Drying is performed in the stoichiometric reactor (R-Stoic) where stoichiometry of reaction and conversion rate are specified. But the reaction kinetic is not necessary to be defined. Next, the gasification is performed in decomposition and gasifier reactors by demonstrating indirect heating at low pressure. Decomposition reactor is simulated by

RYield type reactor which operate at temperature and pressure about of 394 K and 1 atm, respectively. This type of the reactor is modeled by defining the conversion yield of the reaction products and implemented when the stoichiometry and kinetics of the reaction are not known. In this step, the biomass is converted to the C, H<sub>2</sub>, OS, S, N<sub>2</sub> and ash. The gasifier is modeled by using R-Gibbs type of the reactor for combustion at temperature and pressure about of 1100 k and a 1 atm, respectively. The volatile component and syngas production are done by assuming

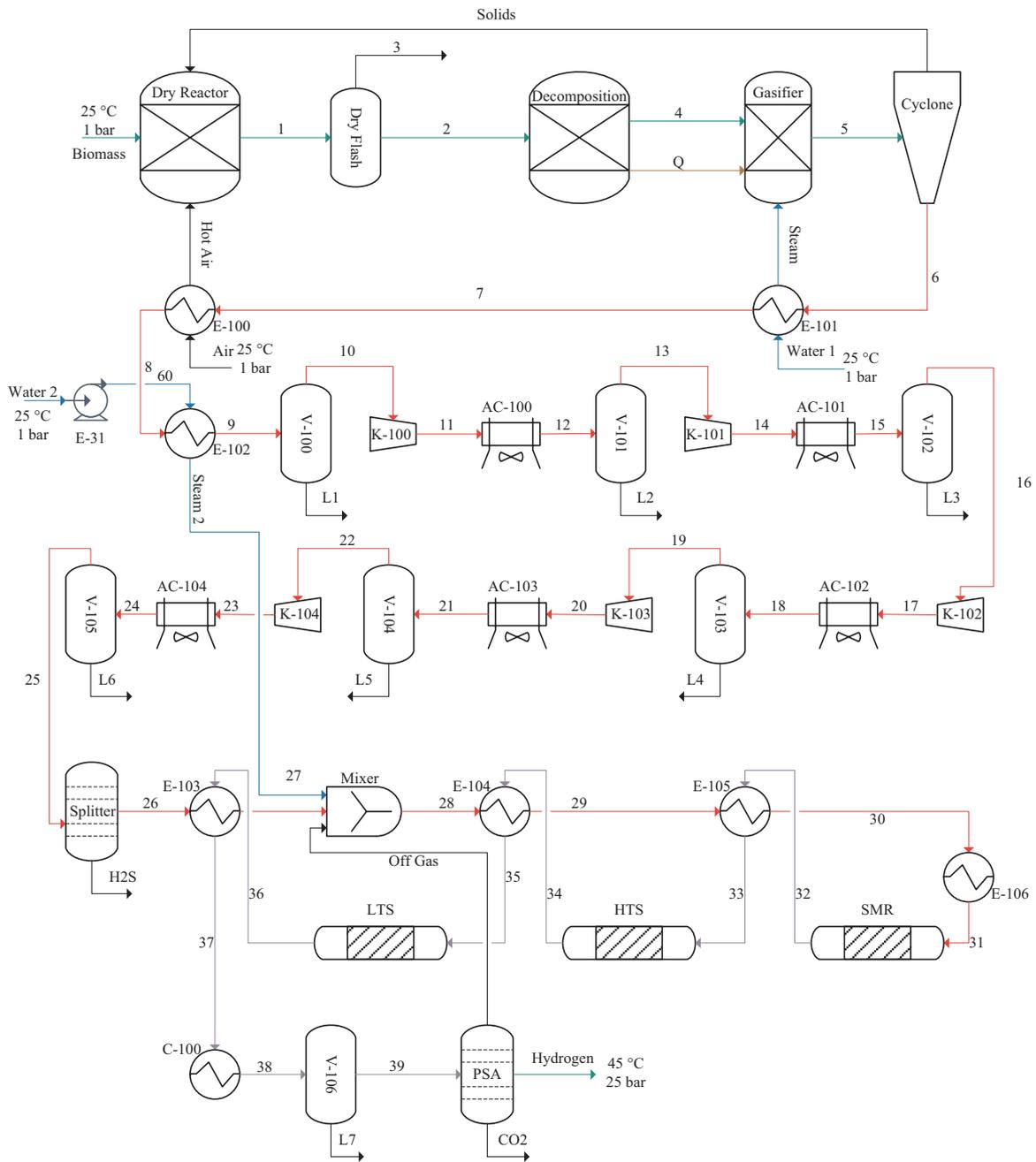


Fig. 14. Process flow diagram of the H<sub>2</sub> production via WGSR.

Table 9  
The used coefficients in constant specific heat equation [86].

Gas	a'	b'	c'	d'
CO	28.16	$0.1675 \times 10^{-2}$	$0.5372 \times 10^{-5}$	$-2.222 \times 10^{-9}$
CO <sub>2</sub>	22.26	$5.981 \times 10^{-2}$	$-3.501 \times 10^{-5}$	$-7.469 \times 10^{-9}$
H <sub>2</sub> O	32.24	$0.1923 \times 10^{-2}$	$1.055 \times 10^{-5}$	$-3.595 \times 10^{-9}$
H <sub>2</sub>	29.11	$-0.1916 \times 10^{-2}$	$0.4003 \times 10^{-5}$	$-0.8704 \times 10^{-9}$
CH <sub>4</sub>	19.89	$5.2040 \times 10^{-2}$	$1.269 \times 10^{-5}$	$-11.01 \times 10^{-9}$

that, Gibbs free energy minimization and the restricted equilibrium method occur in the gasifier. The R-Gibbs reactor is useful when the temperature and pressure are specified but the stoichiometry of the reaction is unknown. The produced syngas enters the cyclone until the solid particles can be separated from it. The separated solid particle is tar (C<sub>18</sub>H<sub>12</sub>). The tar along with vapor components at a temperature of

473 K enters the next combustion reactor where the tar reacted with water vapor to produce C and syngas. For compression of the syngas, the five-stage centrifugal compressor with aftercooler and knock-out drum at each stage is used. The polytropic and mechanical efficiency of the compressor is about 79.0% and 95.0%, respectively. The pressurized syngas at pressure about of 31 atm enters the splitter for purification. In the splitter, the toxic component likes H<sub>2</sub>S is separated from syngas. The purified syngas at high temperature participates in the reactions (52) to (54).



The syngas is mixed with superheat steam and enters the SMR

**Table 10**  
The standard chemical exergy of the biomass components [96,97].

Component	Standard chemical exergy (kJ/kmol)	Enthalpy of formation (kJ/kmol)
H <sub>2</sub> O (vapor)	11710	- 241.82
H <sub>2</sub> O (liquid)	3120	- 285.8
N <sub>2</sub>	690	0
O <sub>2</sub>	3970	0
CO <sub>2</sub>	20140	- 393.5
SO <sub>2</sub>	303500	- 296.8
H <sub>2</sub>	238490	0
CO	275430	- 110.5
H <sub>2</sub> S	804770	- 20.5
NH <sub>3</sub>	341250	- 46.1
NO <sub>2</sub>	56220	+ 33.2
CH <sub>4</sub>	836510	- 74.87
C	410820	0
S	598850	0
Tar	1.01E + 07	- 145.30

reactor. The thermodynamic condition of the reforming is at temperature and pressure about of 1031 K and 24 atm, respectively. Because the methane conversion is decreased at high pressure. Next, the syngas getting cold to temperature about of 667 K and enters the HTS reactor. In the HTS reactor, the CO content is decreased and consequently leads to increase in H<sub>2</sub> production yield. The outlet stream from HTS reactor is cooled to a temperature about of 473 K and enters to LTS reactor. The outlet stream from LTS reactor has the highest value of the H<sub>2</sub>. The WGSR take places at two reactors which are HTS (643–693 K) and LTS (473–523 K). The SMR, HTS and LTS reactors are modeled by RPlug reactor. This type of reactor is suitable when kinetics of the reactions is specified. The produced H<sub>2</sub> enters the separation section. In this section, unreacted syngas which mainly consists of CO, CO<sub>2</sub>, CH<sub>4</sub> and other hydrocarbons is speared by using PSA unit.

7.1. Effect of the biomass type on hydrogen production yield

Different types of the biomass feedstocks result different product and composition when used in the gasification process. In this regard, 23 different biomass are utilized for investigation of the hydrogen production yield in the proposed process. Table 14 shows the calculated

**Table 11**  
The exergy values of the process streams.

Stream no.	Physical exergy (kW)			Chemical exergy (kW)			Total exergy (kW)		
	Rice husk	Larch wood	Wood chip	Rice husk	Larch wood	Wood chip	Rice husk	Larch wood	Wood chip
1	558	6222	1102	347351	527854	371876	348293	534076	372978
2	545	5481	857	347735	529754	371876	348280	535235	372733
3	13	741	244	0	110	445	13	850	689
4	39046	43999	8583	285793	290832	358661	324839	334831	367244
5	22248	23639	19797	308025	313556	310476	330273	337195	330273
6	19953	20716	19421	265444	269315	275179	285398	290031	294599
7	2295	2923	377	86282	109900	14168	88577	112823	14545
8	2474	2780	2402	69091	82794	16637	71565	85574	19039
9	135	266	0	20054	36279	0	20189	36545	0
10	2339	2514	2402	58785	62973	16637	61124	65487	19039
11	8505	9224	8002	304319	306710	316553	312824	315934	324556
12	1679	2185	1346	330981	332408	345222	332660	334593	346568
13	1022	1457	749	334345	335672	348851	335367	337129	349600
14	135	593	3	356325	536538	418360	356636	537130	418363
Biomass	0	0	0	336140	493240	418360	336140	493240	418360
Air	0	0	0	108	108	108	108	108	108
Hot Air	190	190	190	108	108	108	298	298	298
Water1	0	0	0	650	650	650	650	650	650
Steam1	4801	4801	4801	6168	6168	6168	10969	10969	10969
Water2	0	0	0	578	578	578	578	578	578
Steam2	3295	3295	3295	5114	5114	5114	8409	8409	8409
Syngas	68930	3069	1985	386716	392425	360205	455646	395494	362190

**Table 12**  
Definitions of the exergy efficiency of the process components [99].

Components	Exergy destruction	Exergy efficiency
Reactors	$\dot{I} = \dot{E}x_i + \dot{E}x_{Q_i} - \dot{E}x_o - \dot{E}x_{Q_o}$ [101]	$\epsilon = \frac{\sum(\dot{m}e)_o + \dot{E}x_{Q_o}}{\sum(\dot{m}e)_i + \dot{E}x_{Q_i}}$ [102]
Heat exchanger	$\dot{I} = \dot{E}x_i - \dot{E}x_o$ [99]	$\epsilon = \frac{\sum(\dot{m}e)_o}{\sum(\dot{m}e)_i}$ [99]

H<sub>2</sub> production yields. As can be seen, hydrogen yield is higher in biomass with higher total carbon and hydrogen and lower moisture content.

8. Summary and conclusions

In this study, model of the biomass gasification process was simulated for 23 different kinds of the biomass sources. The effect of the operating parameters which are biomass and steam flow rate and RGIBBS reactor temperature was investigated based on the steam biomass gasification process. Energy and exergy analyses along with related expressions development were done for the gasification process and its component. The obtained results indicate that, the maximum syngas energy efficiency refers to Rice husk and Peach stone biomasses. The highest H<sub>2</sub> production yield refers to Rice straw, corn cob and straw biomasses. So, the H<sub>2</sub> rate for production of the syngas is maximum for rice husk. Increasing in biomass quantity leads to an incremental growth in the produced H<sub>2</sub>'s mole fraction. While increasing in steam and gasification process temperature decreases the produced H<sub>2</sub>'s mole fraction. Exergy efficiency of the gasification process for rice husk, wood chip and larch wood was calculated. Regarding the results, the drying reactor has the highest exergy efficiency. Also, exergy destruction rate in the heat exchangers is lower than the other process components. In general, the objectives which can serve as a design criterion for development of the biomass gasification processes for hydrogen production are as follows:

- Based on the the thermodynamic parametric study and first and second laws of thermodynamics, biomass gasification hydrogen production process can be considered as a convenient and noticeable option.

**Table 13**  
Results of the exergy analysis.

Components		Exergy destruction (KW)			Exergy efficiency		
		Rice husk	Larch wood	Wood chip	Rice husk	Larch wood	Wood chip
Reactors	Dry Reactor	8641	3352	45683	98	99	89
	Decomposition	23788	20751	5837	93	63	98
	Gasifier	5717	8524	47859	98	97	87
	Tar combustion	25222	35460	3716	88	84	99
Heat exchangers	E-100	6646	6690	6617	67	68	66
	E-101	3531	3744	3361	58	59	58
	E-102	468	538	408	72	75	70

**Table 14**  
The H<sub>2</sub> production yield via WGS for 23 different types of the biomasses.

Type biomass	Cedar wood	Wood sawdust	Olive oil residue	Rice husk	Rice straw	Pine sawdust
$\eta_{H_2}$	0.14	0.11	0.17	0.14	0.06	0.17
Type biomass	Spruce wood pellet	Coffee husk	Coffee ground	Larch wood	Grapevine pruning waste	Jute stick
$\eta_{H_2}$	0.15	0.10	0.13	0.14	0.11	0.14
Type biomass	Sugar-cane bagasse	Corn cob	Peach stone	Wheat straw	Cotton stem	Straw
$\eta_{H_2}$	0.13	0.06	0.17	0.09	0.09	0.07
Type biomass	Camphor wood	Beech wood	Switch grass	oil palm shell	wood chip	
$\eta_{H_2}$	0.08	0.14	0.12	0.05	0.15	

- The amount of produced hydrogen for different biomasses is between 50 and 170 gr per kg of biomass. Where, the amount of moisture and the components composition, including hydrogen and carbon, affect the amount of the produced hydrogen.
- The biomass gasification efficiency for H<sub>2</sub> production in the entire range of effective parameters presents a high potential.
- Among effective parameters, controlling the gasification temperature and adjusting the ratio of H<sub>2</sub>/CO have a significant effect on the syngas production.
- The syngas production cost can be decreased by implementing a thermochemical method. So, it is necessary to make a comparison between these two methods.
- A detailed study on the effects of catalysts at various stages of H<sub>2</sub> production should be done. A better catalyst can maximize the production efficiency along with lower costs.
- Cost and economic potential analyses of the hydrogen production from biomass gasification should be done in order to make it possible for integration with other thermal processes.
- Blending the other type of the fuels with biomass for co-gasification may increase the H<sub>2</sub> production yield. Therefore, a thermodynamic analysis for choosing the type of fuel and its portion should be done.
- A more accurate study about the internal mass and heat transfer of solid particles between the phases, materials and gasifier boundaries wall can also be investigated.

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