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Simulation of a Downdraft Gasifier for Production of Syngas from Different Biomass Feedstocks

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Abstract: In the evaluation of gasification processes, estimating the composition of the fuel gas for different conditions is fundamental to identify the best operating conditions. In this way, modeling and simulation of gasification provide an analysis of the process performance, allowing for resource and time savings in pilot-scale process operation, as it predicts the behavior and analyzes the effects of different variables on the process. Thus, the focus of this work was the modeling and simulation of biomass gasification processes using the UniSim Design chemical process software, in order to satisfactorily reproduce the operation behavior of a downdraft gasifier. The study was performed for two residual biomasses (forest and agricultural) in order to predict the produced syngas composition. The reactors simulated gasification by minimizing the free energy of Gibbs. The main operating parameters considered were the equivalence ratio (ER), steam to biomass ratio (SBR), and gasification temperature (independent variables). In the simulations, a sensitivity analysis was carried out, where the effects of these parameters on the composition of syngas, flow of syngas, and heating value (dependent variables) were studied, in order to maximize these three variables in the process with the choice of the best parameters of operation. The model is able to predict the performance of the gasifier and it is qualified to analyze the behavior of the independent parameters in the gasification results. With a temperature between 850 and 950 °C, SBR up to 0.2, and ER between 0.3 and 0.5, the best operating conditions are obtained for maximizing the composition of the syngas in CO and H₂.

Keywords: biomass gasification; downdraft gasifier; process simulation; UniSim Design

1. Introduction

Fossil fuels are still the main sources of energy used worldwide, due to their high energy efficiency. However, in addition to the pollution caused by the gases released, fossil energy is finite, being currently depleted fast, boosting the search and the need to use renewable energies [1]. Under this context, solid biomass shows great potential to become an energetic alternative to fossil energy sources. This renewable energy is abundant and has a virtually zero carbon dioxide (CO₂) balance since the CO₂ produced in power generation is equivalent to the CO₂ consumed during the growth of the plant from which the biomass was originated [2].

Biomass is a source of energy that can potentially be obtained from forest-related industrial wastes, such as wood chips and sawdust, as well as from agricultural wastes, such as rice husk, straw, and sugarcane bagasse [3–6]. The amount of forest waste in Portugal is approximately 2.2 million tons per year. Portugal is the European country with the highest number of forest fires and the second with the most burned area. Most of the fires are caused by the use of fire to burn trash and waste. Thus, the use of forest biomass for energy production can minimize the damage to landowners, forest neighbors, and investors, as it provides a destination for waste, produces energy, and tends to reduce fires [2,7,8].



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Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). Biomass gasification is the conversion of organic materials into an energetic gas, rich in hydrogen (H₂) and carbon monoxide (CO), through oxidation and reduction reactions at elevated temperatures. In the evaluation of gasification processes, estimating the composition of the fuel gas for different conditions is fundamental to identify the best operating conditions. In this way, gasification modeling and simulation provide an advance virtual analysis of the process performance, allowing for resource and time savings in pilot-scale process operations, as it predicts the behavior and analyzes the effects of different variables on the process [9–14].

Thus, the focus of this work is the modeling and simulation of biomass gasification processes using the UniSim Design chemical process software, applying the tools available in the simulator database in order to satisfactorily reproduce the operation behavior of a gasifier. The work is associated with a parallel project concerning the design, construction, and test of a pilot downdraft gasifier, aiming for the energetic valorization of residual biomass from fire-hazard areas. So, the developed model is focused specifically on the production of syngas from complex sources represented by mixtures of carbon rich organic wastes, which can show a variety of compositions. Hence, the chosen simulated gasifier has a downdraft design and it will be studied for the processing of forest and agricultural waste type biomasses. Optimization and sensitivity analysis will be performed to observe the influence of significant parameters affecting the process (e.g., equivalence ratio, steam to biomass ratio, and temperature) on the properties of the synthesis gas produced (e.g., composition and heating value).

This gas is a mixture composed mainly of carbon monoxide (CO), hydrogen (H₂), and methane (CH₄). The gas produced can be standardized in quality and is easier and more versatile to use than the original biomass, either for fueling gas engines and gas turbines or as a chemical raw material for liquid fuel production [15]. Gasification adds value to low or negative value raw materials by converting them into fuels. This conversion process is more complex than simple combustion and is influenced by many factors, such as amount of oxidant, feedstock composition, gasifier temperature, and reactor geometry [16,17].

The main gasification reactions are shown in Table 1 [3,4,14,16,18,19].

Gasification Step	Reaction		ΔH° (kJ/mol)
Pyrolysis	$Biomass \rightarrow Ch$		
Oxidation	$\begin{array}{c} Char(s)+O_2\rightarrow CO_2\\ C(s)+0.5O_2\rightarrow CO\\ CO+0.5O_2\rightarrow CO_2\\ H_2+0.5O_2\rightarrow H_2O \end{array}$	Carbon Oxidation (2) Carbon Partial Oxidation (3) Carbon Monoxide Oxidation (4) Hydrogen Oxidation (5)	-394 -110 -283 -242
Reduction	$\begin{array}{c} C(s) + CO_2 \leftrightarrow 2CO\\ C(s) + H_2O \leftrightarrow CO + H_2\\ CO + H_2O \leftrightarrow CO_2 + H_2\\ C(s) + 2H_2 \leftrightarrow CH_4\\ CH_4 + H_2O \leftrightarrow CO + 3H_2 \end{array}$	Boudouard Reaction (6) Reforming of Char (7) Water Gas Shift Reaction (8) Hydrogasification (9) Steam-methane Reforming (10)	172 131 -42 -75 206

Table 1. Main reactions involved in the gasification processes.

The downdraft gasifier design (see Figure 1) is a reactor where the solid material is inserted in the top and the oxidizing gas enters the reactor laterally above the grid. The gasifying agent is introduced directly into the combustion zone, then flows into the reduction zone, and is extracted from the gasifier. The synthesis gas exits the gasifier after passing through the hot zone, allowing partial cracking of the tars formed during gasification, which provides a gas with low tar. However, the gases leave the gasifier at high temperatures (900–1000 $^{\circ}$ C), leading to low efficiencies, due to the high heat content carried by the hot gas. This reactor is suitable to convert biomass with high volatile content, but it is limited in scale. It also needs specific biomass conditions and is not suitable for various types of biomass [9,16].



Figure 1. Downdraft gasifier.

In computer simulation, the processes and equipment operate following the sequence of input data, data processing, and return output data. Usually, these data are mass flows, temperatures, compositions, and pressures. For the construction, adaptation, or scaling of equipment, it is necessary to obtain well-dimensioned parameters. If these actions are done without prior study, the experimental data obtained may not be satisfactory and time and money have been spent on incorrect reactor sizing and operation [20,21].

Modeling and simulation of gasification systems help in predicting the outlet gas composition when operating conditions and scale size change. This assists in planning the construction or retrofitting of existing equipment. UniSim Design is a chemical process modeling software, with a similar design to that of Aspen Plus and Aspen Hysys. It is used in engineering to create dynamic and steady-state models for plant design, monitoring, troubleshooting, planning, and management. It is possible to build simulation processes in an integrated graphical environment including tools that allow the optimization of these processes.

In the literature, there are studies of modeling and simulation of biomass gasification mainly using Aspen Plus and Aspen Hysys [1,2,4,18,22–27]. In this work, UniSim Design will be used as an alternative software for these applications. A small-scale gasifier will be modeled and simulated, in order to process several types of forest biomass and agricultural wastes, thus giving a purpose to this residue. The type of gasifier chosen is a downdraft due to the simple design, low cost, and quality of the outlet gas. Additionally, a nonstoichiometric equilibrium model is assumed considering that the reaction system is in its most stable state (lowest free energy). For this, the main hypothesis presumed is that the gasification reaction rates are fast enough and the residence time is long enough to reach equilibrium. This condition is met at gasification temperatures above 800 °C. Thus, the largest discrepancies between estimated and experimental values are found at low temperatures, where the CO and H_2 fractions are overestimated and the CO₂ and CH₄, tar, and residual carbon fractions are underestimated. This model is based on minimizing Gibbs free energy to determine the product composition obtained and the efficiency of the gasifier. The advantage of this method is that there is no need for the establishment of a specific set of reactions to solve the problem, requiring knowledge of only the approximate and ultimate analysis [11].

Regardless of the software used for modeling and simulation of the gasification process, there is a pattern of steps that must be followed in order to successfully perform the simulation. These steps represent the four main zones present in a downdraft gasifier, namely: drying, pyrolysis, oxidation, and reduction zones. Therefore, the simulation consists of several unit operation blocks and, as in this work, the process is divided into three blocks: drying and decomposition, combustion, and gasification. In the drying and decomposition block, the moisture content is reduced, and the biomass is decomposed into volatile and char compounds. In the combustion and gasification block, the oxidation and reduction reactions will be modeled, minimizing Gibbs free energy. The approach will be non-stoichiometric, requiring the specification of the ultimate and approximate biomass composition and the reactions involved in the process.

Chemical engineering software provides databases for conventional fluids and solids properties. Therefore, when unconventional materials such as biomass are employed, a strategy should be used to inform the software about the composition of the material entering the process. The strategy that will be used in this work is to consider biomass as a generic char material. This allows, from the approximate and ultimate analysis of the material, the calculation of the properties of this unconventional material, hence, obtaining the feed stream characteristics.

The next step is the drying and decomposition block, where the goal is to reduce the moisture content of the biomass and the dried material will be converted into components such as carbon, hydrogen, oxygen, nitrogen, and ashes, specifying the distribution according to the ultimate and approximate analysis.

Finally, there is the combustion and gasification stage, where a Gibbs reactor will be used to minimize Gibbs free energy by calculating the gas composition reaching full chemical equilibrium. In this block, air will be introduced as a gasification agent. Upon exiting this reactor, the gas produced will pass a separating block that will remove water. Therefore, the gaseous output stream obtained from this separator contains the desired syngas at the end of the process.

2. Simulation Model

A gasification model was constructed in UniSim Design. In this process, a series of unit operations were selected, integrated, and sequenced in order to simulate the entire process.

2.1. Assumptions

Some considerations were made for the construction of this model considering a downdraft gasifier configuration:

- 1. The process operates in steady state;
- 2. The operation takes place at atmospheric pressure and all pressure losses are neglected;
- 3. The produced char is 100% carbon;
- 4. Peng–Robinson equation of state was selected as the thermodynamic package for the whole process;
- 5. Air consists of 79% N₂ and 21% O₂ on a molar basis;
- 6. N₂ is a diluent and an inert gas, so it does not react;
- 7. Sulfur (S) and chlorine (Cl) bounded to the fuel are converted in hydrosulfuric acid (H₂S) and hydrochloric acid (HCl), respectively;
- 8. Since the temperature conditions can be very different in the two reaction zones (combustion and reduction), even for small scale gasifiers, these reaction zones are simulated using two different reaction systems;
- 9. The formation of tar is significantly reduced in the process, so it is neglected during the simulation; therefore a sufficiently high temperature is fixated in the combustion zone (1000 °C) to account for a reasonable tar degradation yield;
- 10. The reduction reaction zone is simulated using two Gibbs reactors in series, operating adiabatically.

2.2. Feedstock

The selected biomass sources were hardwood chips and almond shells, considered as a hypothetical char simulated from the parameters shown in Table 2. The input values (kg/h) of air and steam are listed in Table 3, in addition to the conditions of process operation.

Table 2. Approximate and ultimate analysis of the biomass stocks [28,29].

Biomass Feedstock		Hardwood Chips	Almond Shells
Approximate analysis (wt.%)			
	Fixed carbon	14.191	15.870
	Volatile matter	79.470	80.280
	Moisture	5.393	3.300
	Ash	0.946	0.550
Ultimate analysis (wt.%)			
-	Carbon	49.316	50.500
	Hydrogen	5.902	6.580
	Nitrogen	0.150	0.210
	Oxygen	44.614	42.654
	Sulfur	0.015	0.006
	Chlorine	0.003	0.050
Higher calorific value (MJ/kg)		17	18
Flow rate (kg/h)		5	5

Table 3. Input parameters in the simulation study.

Air Feedstock		
Temperature	25	°C
Flow rate	0.3–2.4	kg/h
Steam Feedstock		
Temperature	100	°C
Flow rate	0.18–3.6	kg/h
Operating conditions		
Temperature	600-1200	°C
Pressure	1	atm

2.3. Simulation Basis Manager

The Simulation Basis Manager (SBM) is the interface of the simulation project in UniSim Design, where the components are selected and/or constructed, packages of fluid properties are chosen in order to assist the execution of the calculations, and sets of chemical reactions are defined. All the data can be incorporated into the unit operations which define the equipment that constitutes the process. UniSim Design does not consider any form of biomass as a predefined component in its component library. In this way, the composition of biomass was modeled by Python software using the ultimate and approximate analysis to estimate the properties of the decomposed input stream. The mass and molar composition values of the biomass for complete decomposition are shown in Table 4.

	Hardwo	od Chips	Almond Shells		
Composition (%)	Mass	Molar	Mass	Molar	
C	49.316	49.618	50.500	48.227	
O ₂	39.552	14.937	39.723	14.239	
H ₂	5.263	31.550	6.209	35.328	
N ₂	0.150	0.065	0.210	0.086	
H_2S	0.016	0.006	0.006	0.002	
HC1	0.003	0.001	0.052	0.017	
H ₂ O	5.700	3.823	3.300	2.101	

Table 4. Mass and molar composition of the decomposed biomass.

2.4. Sensitivity Analysis

In this section will be studied the sensitivity of the model developed for a downdraft gasifier. The syngas at the end of the process must be formed by CO, H_{2} , and variable amounts of CH₄, H_2S , HCl, and N_2 . The sensitivity analysis focuses on studying the effect of the equivalence ratio (ER), steam to biomass ratio (SBR), and gasifier temperature on the following variables: molar composition of syngas, flow of syngas, and heating value.

2.5. Model Description

The process is simulated in three main steps: drying and decomposition, combustion, and gasification. For this, a conversion reactor, Gibbs reactors, as well as other equipment such as mixers and splitters were used. The flow sheet is illustrated in Figure 2.





2.5.1. Drying and Decomposition

The input stream "Biomass" was defined by Python software from the ultimate and approximate analysis, shown in Table 4. This stream enters at 500 °C in the splitter equipment, named "Water Splitter" to separate the water present in the biomass, leading thus to the streams "Dry Biomass" and "Water".

Another Splitter equipment, named "Volatile Splitter" was used to separate volatile materials from char, obtaining the streams "Volatile Materials" and "Char". After that, the "Volatile Materials" stream enters another Splitter equipment, named "Acid Splitter" where the acids present in the volatile materials are separated. Thus, at the end of this block the currents "Volatile Feed", "Char", "Acid Gases", and "Water" are obtained.

2.5.2. Combustion

This block is where the combustion reactions are simulated: carbon oxidation (2), carbon partial oxidation (3), carbon monoxide oxidation (4), and hydrogen oxidation (5), according to Table 1. For this, a conversion reactor equipment was used, named "Combustor", which is operated at 1000 °C, which was considered a sufficiently high value

in order to ensure a reasonable tar degradation yield. The input streams in this equipment are "Volatile Feed", "Char", "Air" and "Combustor Duty". From this equipment, the streams "Flue Gases" and "Comb Bottom" are obtained.

2.5.3. Gasification

Gasification reactions are a set of equilibrium reactions. To facilitate modeling in UniSim Design, the set of reactions was separated into two Gibbs reactors. Both reactors operate adiabatically for the whole analysis with the exception of the study presented in Section 3.4, where the influence of the gasification temperature is assessed. For feeding in the first reactor, mixer equipment, named "Mix", was used to mix the following streams: "Flue Gases", "Comb Bottom", "Acid Gases", and "Water", thus obtaining a unique stream named "To Gasif" that enters the first Gibbs reactor named "Gibbs Gasificator". The following reactions are considered in this reactor: Boudouard reaction (6), reforming of char (7), and hydrogasification (9), according to Table 1. The first two reactions are endothermic and the third one is exothermic. The streams exiting this reactor are "Gasif Gases" and "Gasif Bottom", both of which enter the next reactor, in addition to the "Steam" stream inlet.

In the second reactor, named "CO Shift", two reactions are modeled: water gas shift reaction (8) and steam–methane reforming (10), according to Table 1. The first reaction is exothermic and the second one is endothermic. From this reactor, two streams are removed: "Product Gases", which enter the next equipment, and the "Solid Bottom" stream. Finally, there is a "Splitter" device, named "Syngas Splitter" that simulates the removal of water from the gas. This equipment has as input stream "Product Gases" and as output two streams: "Water" and "Syngas". The "Syngas" being the final stream, thus obtaining the product gas at the end of the process.

3. Results and Discussion

3.1. Reference Conditions

The syngas at the end of the process must be formed by CO, H_{2} , and small amounts of CH₄, H_2S , HCl, and N_2 . After gathering the simulated data, the model developed for a downdraft gasifier will be compared with two case studies selected from the literature [28,30].

3.1.1. Simulation

Considering the developed model, base simulation runs were performed with each of the two selected biomass sources (hardwood chips and almond shell). In this simulation, the steam to biomass ratio (SBR) chosen was 0.2 for both biomass. The chosen equivalence ratio (ER) was 0.4 for hardwood chips and 0.45 for almond shells, in which air entered the process at 25 °C and steam at 100 °C as shown in Table 5.

Almond Shells Hardwood Chips Air Steam Air Steam ER 0.40 0.45 SBR 0.20 0.20 25.0 25.0 Temperature (°C) 100.0 100.0 0.042 Molar flow (kmol/h) 0.0550.0450.055 Mass flow (kg/h) 1.296 0.991 1.405 0.991

Table 5. Parameters considered in the base simulations.

In Tables 6 and 7 are presented the main process streams, temperatures, flows (molar and mass), syngas heating values, and molar compositions. The decomposed inlet stream "Biomass" enters the process at 500 °C with a mass flow of 5 kg/h with the compositions determined from the ultimate and approximate analysis using the Python software, having a high composition of C, O_{2} , and H_2 . The "Flue Gases" stream is the equipment's output

that simulates oxidation reactions. It is observed that the stream leaves the equipment with a fixed temperature of 1000 $^{\circ}$ C. It is interesting to note that the main reaction favored was carbon partial oxidation (3), due to the low intake of air, favoring the formation of CO. The other reactions are favored when the amount of air for combustion is higher.

	Biomass	Flue Gases	To Gasif	Gasif Gases	Product Gases	Syngas
Temperature (°C)	500.0	1000.0	972.5	868.5	788.7	788.7
Molar flow (kmol/h)	0.414	0.329	0.361	0.353	0.412	0.386
Mass flow (kg/h)	5.000	5.819	6.296	6.296	7.287	6.811
HHV (MJ/kg)	-	-	-	-	-	14.632
LHV (MJ/kg)	-	-	-	-	-	13.501
HHV (MJ/m^3)	-	-	-	-	-	2.925
LHV (MJ/m ³)	-	-	-	-	-	2.699
C (molar %)	49.618	0.000	4.426	0.000	0.000	0.000
O ₂ (molar %)	14.937	0.000	0.000	0.000	0.000	0.000
H ₂ S (molar %)	0.006	-	0.007	0.007	0.006	0.006
HCl (molar %)	0.001	-	0.001	0.001	0.001	0.001
H ₂ O (molar %)	3.823	0.000	4.386	0.465	6.408	0.000
CO (molar %)	-	57.570	52.492	56.488	42.063	44.943
H ₂ (molar %)	31.550	39.693	36.192	38.823	41.601	44.449
CO ₂ (molar %)	-	0.000	0.000	0.579	7.319	7.819
CH ₄ (molar %)	-	-	-	1.085	0.419	0.448
N ₂ (molar %)	0.065	2.738	2.496	2.551	2.184	2.334

Table 6. Main simulation streams for hardwood chips.

Table 7. Main simulation streams for almond shells.

	Biomass	Flue Gases	To Gasif	Gasif Gases	Product Gases	Syngas
Temperature (°C)	500.0	1000.0	984.8	938.5	805.2	805.2
Molar flow (kmol/h)	0.436	0.359	0.383	0.371	0.435	0.410
Mass flow (kg/h)	5.000	6.059	6.405	6.405	7.396	6.943
HHV (MJ/kg)	-	-	-	-	-	15.477
LHV (MJ/kg)	-	-	-	-	-	14.253
HHV (MJ/m^3)	-	-	-	-	-	2.923
LHV (MJ/m ³)	-	-	-	-	-	2.692
C (molar %)	48.227	0.000	3.869	0.000	0.000	0.000
O ₂ (molar %)	14.239	0.000	0.000	0.000	0.000	0.000
H ₂ S (molar %)	0.002	-	0.002	0.003	0.002	0.002
HCl (molar %)	0.017	-	0.018	0.019	0.016	0.017
H ₂ O (molar %)	2.101	0.000	2.389	0.084	5.781	0.000
CO (molar %)	-	54.392	50.976	54.930	42.028	44.606
H ₂ (molar %)	35.328	42.868	40.176	40.536	43.625	46.301
CO ₂ (molar %)	-	0.000	0,000	0.080	5.921	6.284
CH ₄ (molar %)	-	-	-	1.693	0.365	0.387
N ₂ (molar %)	0.086	2.741	2.569	2.656	2.263	2.402

In the stream "To Gasif" all the previous streams are joined together to enter the first reactor that simulates the reduction reactions. The temperature in the stream "To Gasif" decreases slightly in relation to the stream that leaves the combustion equipment, due to the lower temperatures of the other streams, entering in thermal equilibrium. This stream contains the char that has not been volatized, the acid gases, in addition to the stream that comes from the combustor. Therefore, an amount of C is noted, due to the char, the presence of water, due to the biomass moisture, and also the gases already formed before $(CO, H_2, and inert N_2)$.

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The "Gasif Gases" stream is the output of the first equipment that simulates the reduction reactions. In this stream, it is noted that there was an increase in the composition of CO, in addition to the formation of CH₄ and all consumption of C. This is due to the favoring of reactions such as reforming of char (7) and hydrogasification (9). The reaction (9) is exothermic and the reaction (7) endothermic, however the reaction of reforming of char has an enthalpy 2.3 times higher, thus the temperature in this area of the gasifier is lower in relation to the inlet stream because there was a higher consumption of energy compared to the energy released by the exothermic reaction.

The stream "Product Gases" is the outlet stream of the second gasifier reactor "CO Shift" that simulates the reduction reactions. It is observed that the temperature has declined in relation to the inlet stream. It is also noted that there was a rise in the composition of H_2 and CO_2 , and a reduction in the composition of CH_4 and CO. This behavior is due to the fact that the steam entering the gasification step "CO Shift" favors the water gas shift reaction (8) and steam–methane reforming (10) reactions, consuming CO, CH_4 and H_2O , to form mostly H_2 and CO_2 . A possible explanation for the decrease in temperature is that, in spite of reaction (8) being exothermic, reaction (10) is endothermic with an enthalpy five times higher. In addition, the steam enters at 100 °C, so the reaction temperature is expected to diminish through the establishment of a thermal equilibrium. The behavior of the variations, both of the compositions and of the temperatures, was similar for the two biomasses. The "Syngas" outlet stream has high compositions of CO and H₂, close to 45%, and low compositions of the other components (H_2S , HCl, CH_4 , and N_2). Only CO₂ showed a formation between 6 and 7%. However, with the steam inlet, it is inevitable to favor the water gas shift reaction (8) and consequently the formation of CO_2 . The feed of steam promotes the formation of H_2 , but it also has the problem of favoring the formation of CO_2 . Therefore, it is advisable to work with a low steam value in order to avoid this difficulty.

3.1.2. Literature

The results of two studies of biomass gasification reported in the literature [27,29], one regarding the gasification of hardwood chips and the other of almond shells, are here presented and discussed, to be compared to the study performed in this work (Table 8).

Studies	Model 1 [27]	This Work Model	Model 2 [29]	This Work Model
Type of biomass	Hardwood chips	Hardwood chips	Almond shells	Almond shells
Type of gasifier	Downdraft	Downdraft	Fluidized bed	Downdraft
Gasifying agent	Air	Air and steam	Air and steam	Air and steam
Software	Aspen Plus	UniSim Design	UniSim Design	UniSim Design
Pressure (atm)	- 1	1	1–3	1
Temperature (°C)	500-1000	600-1200	700-1100	600-1200
Moisture (%)	8.91	5.39	3.30	3.30
ER	0.20-0.45	0.10-0.80	0.00-1.00	0.10-0.80
SBR	_	0.00-0.75	0.44 - 1.00	0.00-0.75
CO (%)	21.31 (41.54) *	44.94	59.60	44.61
H ₂ (%)	18.29 (35.58) *	44.45	23.18	46.30
CO ₂ (%)	11.36 (22.48) *	7.82	0.01	6.28
CH4 (%)	0.20 (0.39) *	0.45	6.12	0.39
N ₂ (%)	48.99 (0.00) *	2.33	8.29	2.40

Table 8. Parameters and results of reference studies [27,29].

* N2-free basis.

Regarding the simulation of almond shells gasification, the gasifier selected was a fluidized bed gasifier [29]. The gasifying agent used was air and steam. The study was also carried out using the chemical processes simulation software UniSim Design. The pressure varied between 1 and 3 atm and the temperature ranged between 700 and 1100 °C. In the analysis of air intake, a decrease in CO and H₂ was observed with a rise in

air flow. The ER varied between 0.00 and 1.00. Another parameter analyzed was steam added to the process: SBR varied between 0.44 and 1.00, and an increase in the steam feed led to a reduction of the CO composition and to a rise of the H₂ composition. Additionally, it was observed that the composition of CO and H₂ in the syngas stream increased with temperature value.

The simulation of the gasification of hardwood chips was carried out in a downdraft gasifier [27]. The gasifying agent used in the process was just air. The study was done using Aspen Plus. The pressure was fixed at 1 atm and the temperature varied between 500 and 1000 °C. In the analysis of air intake, the compositions of CO, H₂, and CH₄ in the syngas were found to decrease with the rise of ER, while the composition of CO_2 increases with the rise of ER. The ER varied between 0.20 and 0.45. In relation to the growth in the gasifier temperature, the composition of the syngas increased in CO and decreased in CO₂ and CH₄. H₂ behaved in such a way that its value increased until the temperature of 750 °C and after that, the composition of H_2 declined. It is concluded that the recommended temperature for the gasification is between 650 and 800 °C and that the equivalence ratio is between 0.2 and 0.3 to obtain the best syngas composition parameters. Although the biomasses are of different sub-classifications (forestry residues and agricultural solid waste), they are similar in relation to the composition (ultimate and approximate analysis), so a similar behavior is expected for the final composition of the syngas. If the syngas composition obtained with the hardwood chips is presented in a N₂-free basis, the amount of CO would be 41.54%, H₂ 35.58%, CH_4 0.39%, and CO_2 22.48%. As excess air was used to obtain this syngas stream, a considerable amount of CO_2 was produced. It would be interesting to work with a low air intake to avoid the production of CO_2 and the presence of N_2 in the outlet composition of the synthesis gas produced.

Table 8 shows that the outlet gas compositions diverged from those obtained in the almond shell study, where the amount of CO was higher (approximately 30%) compared to our study, while the amount of H₂ was lower (approximately 50%). It may be due to the fact of considering a low amount of steam. The study with hardwood chips was closer in terms of composition. In a N₂-free basis composition, it should be noted that CO differs 8% and H₂ 20%. It is also seen that there is a large amount of CO₂ (22.48%), compared to our study (7.82%). As previously discussed, this high presence of CO₂ is due to the fact that a large amount of air is used to carry out the process.

It can be noted that both ER and SBR are parameters that significantly change the composition of the outlet gas. For the simulations that will be presented in the next section, low air intakes were applied in order to avoid formation of CO_2 , in addition to analyzing whether the steam input significantly interferes with the expected syngas composition. Therefore, in the next sections, the sensitivity analysis will be carried out with the focus of studying the effect of the equivalence ratio (ER) and of the steam to biomass ratio (SBR) on the following variables: molar composition of the syngas, flow of syngas (molar and mass), syngas heating value and gasifier temperature; and the effect of the gasifier temperature on the molar composition of the syngas, flow of syngas (molar and mass) and syngas heating value.

3.2. Effect of Equivalence Ratio

In this stage, the study of the influence of the air intake on the composition of syngas, heating value, and gasification temperature is presented. Here the ER is the independent variable, with the molar composition of the syngas, the flow of syngas, heating value, and gasification temperature as dependent variables. For this study, the biomass input is fixed at 5 kg/h, considering the same biomass input in all analyzes. In addition, the air intake was varied up to 2.4 kg/h (approximately 0.8 ER) and there was no steam entry in the process, only the water present in the biomass moisture was used.

3.2.1. Molar Composition of Syngas

The equivalence ratio is defined as the air to biomass ratio required for gasification divided by the stoichiometric ratio required for combustion. As the ER rises, the amount of oxygen supplied to the gasifier also grows, providing a higher conversion of the carbon present in the fuel. However, an excessive amount of oxygen will completely oxidize, leading to the decline of the fuel and the production of syngas. Therefore, ER is an essential parameter in the gasification process [4,12,27,30]. Figure 3 shows the effect of the equivalence ratio on the composition of the synthesis gas for both studied biomasses. The behavior for both biomasses was similar. Initially, the amount of hydrogen increases, methane decreases, due to the favoring of hydrogen formation reactions, namely reforming of char (7), water gas shift reaction (8), and steam-methane reforming (10). In addition to the fact that carbon monoxide has a minimal decline, this is also due to the amount of inert N₂ that rises with increasing air intake. However, in the ER close to 0.4, for hardwood chips, and 0.5 for almond shells, the amount of hydrogen stabilizes and begins to decay and the formation of carbon dioxide begins. At this ER value, the amount of oxygen present causes the process to be similar to combustion, with a decrease in H_2 and CO to form CO_2 . Thus, the air intake maximizes gasification in the range of 0.2 to 0.5 of ER, obtaining the highest H₂ values, high CO composition, and virtually zero CO₂ composition. For ER values below 0.2, gasification is incomplete, and above 0.5, gasification is similar to combustion, with the increased formation of CO₂.



Figure 3. Effect of ER on the composition of syngas for hardwood chips (a) and almond shells (b).

3.2.2. Molar and Mass Flow of Syngas

Another important parameter to analyze is the production of syngas. This variable shows the amount of gas that is produced as a function of time. Both molar and mass quantities of this production were studied as a function of the equivalence ratio. As the independent variable is the air intake, the flows were also analyzed in a N₂–free basis. Therefore, Figure 4 shows the behavior of the molar and mass flow as a function of the equivalence ratio for both studied biomasses. It is observed that the mass flow rate increases with the rise of air intake. This is expected because a greater amount of air promotes the formation of H₂ and, for ER values higher than 0.4, the formation of CO₂, in addition to increasing the amount of the inert gas N₂. When N₂ is not considered in the mass flow, there is a reduction of approximately 1% at low ER values and approximately 6% at high ER values. The molar flow increases until approximately an ER value of 0.4, for hardwood chips, and 0.5 for almond shells, after which the molar flow decreases. This can be explained by the fact that from this equivalence ratio there is a decline in the amount of H₂ and a rise in CO₂. As the molar mass of CO₂ is greater than the molar mass of H₂, a

greater mass of CO_2 gas is required to obtain the same molar amount of H_2 . This behavior is observed in the curves at the moment when H_2 starts to decline and CO_2 increases, which is where the molar flow of the synthesis gas starts to decrease. When N_2 is removed from the molar flow, there is a fall in the production of syngas by approximately 1% at low ER values, and 4% at high ER values.



(a) hardwood chips

(**b**) almond shells

Figure 4. Effect of ER on the molar and mass flow of syngas obtained with hardwood chips (a) and almond shells (b).

3.2.3. Heating Value

The heating value of a product gas is a measure of quality. This heating value decreases as more air is supplied [20,31]. Figure 5 shows the behavior of the high and low heating values due to the growth in the equivalence ratio for both studied biomasses. As predicted, both heating values decline with increasing ER (approximately 33% for hardwood and 30% for almond shell). This is due to the fact that the increase of air in the process causes a greater amount of N₂ in the synthesis gas, in addition to favoring the formation of CO₂. If N₂ is removed from the synthesis gas, there is a rise in the heating value (approximately 5% for hardwood and 6% for almond shell). However, the same decreasing behavior is observed when the ER is varied. Therefore, the CO₂ upsurge is the factor that most affects the calorific value. Thus, the heating value of the gas declines with the increase in ER.



(a) hardwood chips

(b) almond shells

Figure 5. Effects of ER on heating values of the synthesis gas obtained with hardwood chips (a) and almond shells (b).

3.2.4. Gasifier Temperature

Usually, the gasification temperature is analyzed as an independent variable depending on the composition of the synthesis gas [6,18]. However, it is interesting to analyze the temperature behavior of the gasifier when considering the temperature as a dependent variable. Figure 6 shows how the temperature in the reactors behave with the growth in the equivalence ratio for the two biomasses analyzed. It can be noted that up to the ER of 0.4, for hardwood chips, and 0.45 for almond shells, the temperature of the gasification declines with the increase of air. It is the behavior expected in gasification since the main reduction reactions are endothermic—Boudouard (6), reforming of char (7), steam-methane reforming (10), consuming the existing heat and causing the temperature to decrease. From that value (0.4 or 0.45), the temperature starts to increase. This is due to the fact that from that ER value, gasification is similar to combustion. Thus, the equilibrium of the hydrogen oxidation reaction shifts to form more water, causing the water gas shift reaction (8) gasification reaction to shift to the formation of CO_2 , causing energy to be released, and thereby increasing the temperature inside the reactor. It is important to highlight that in this ER there is no longer CH_4 , so there is no favoring of the steam–methane reforming (10) reaction, which is endothermic.



(**a**) hardwood chips

(**b**) almond shells

Figure 6. Effect of ER on the temperature of the gasifier operated with hardwood chips (a) and almond shells (b).

3.3. Effect of Steam to Biomass Ratio

The study of the influence of steam input on the composition of syngas, heating value, and gasification temperature was done considering SBR as the independent variable, with the molar composition of syngas, flow of syngas, heating value, and gasification temperature as dependent variables. For this study, the biomass input is fixed at 5 kg/h. In addition, the steam intake was varied up to 3.6 kg/h (approximately 0.7 SBR) and the air intake was fixed at 1.25 kg/h (approximately 0.4 ER).

3.3.1. Molar Composition of Syngas

The steam to biomass ratio is the ratio of the flow of steam to the flow of biomass. This is an important parameter in the gasification process as it is directly linked to the formation of H₂. The steam upsurge in the reactor favors H₂ formation reactions, especially water gas shift reaction (8) and steam–methane reforming (10). However, it also ends up favoring the formation of CO₂. Thus, it is necessary to define the best ratio to not have unwanted amounts of CO₂ in the synthesis gas [17,23,32]. Figure 7 shows the behavior of the syngas composition as the steam to biomass ratio increases. Both biomasses revealed similar behavior. So, the rise in steam causes the amount of carbon monoxide and methane to

decrease. Hydrogen and carbon dioxide, on the other hand, exhibit the opposite behavior, increasing the composition with increasing steam. This is due to the fact that steam favors the water gas shift reaction (8) and steam–methane reforming (10) reactions, consuming CO and CH_4 and forming mostly H_2 and CO_2 .



Figure 7. Effect of SBR on the composition of syngas for hardwood chips (a) and almond shells (b).

3.3.2. Molar and Mass Flow of Syngas

It is also important to analyze the production of syngas in relation to the feeding of steam into the gasifier. Thus, the influence of steam on the molar and mass amount of syngas flow was studied. Figure 8 shows the behavior of the molar and mass flow of syngas as a function of the steam to biomass ratio for the two studied biomasses. Note that both mass and molar production of syngas increase with increasing SBR. This can be explained by the fact that the surge in steam promotes the formation of H₂ and CO₂ mainly because of the water gas shift reaction (8). This causes the mass production to increase with the growth of the SBR. Regarding molar production, the increasing behavior can be explained by the fact that regardless of the SBR value analyzed, the amount of H₂ and CO₂ is always increasing, with no change in the behavior of the molar composition of syngas (CO and H₂), that are always increasing, without increasing and then decreasing in H₂ composition (as seen in the ER study), making also the production of syngas to perform in a similar way.



(a) hardwood chips

(b) almond shells

Figure 8. Effect of SBR on the molar and mass flow of syngas obtained with hardwood chips (a) and almond shells (b).

3.3.3. Heating Value

The heating value of the synthesis gas decreases with the rise of steam in the gasification process [17,33]. As can be observed in Figure 9, the behavior for both biomasses was similar to that found in the literature. As the steam increases, the calorific value decline (approximately 21% for hardwood and 20% for almond shell). This is due to the fact that a higher amount of steam provides a higher amount of CO_2 and a lower amount of CO in the syngas. Even with the rise in the amount of H_2 , this decay of CO makes the internal enthalpy released by the syngas to be lower. The calorific value is defined as the amount of energy produced by the fuel when it burns. The CO oxidation reaction is exothermic, so there is a lower amount of CO in the syngas, which causes the calorific value to decrease. Therefore, a drop in CO and a rise in CO_2 causes the calorific value, both higher and lower, to be lower.





3.3.4. Gasifier Temperature

Analyzing the behavior of temperature as a dependent variable with the growth in the amount of steam in the reactors, it is observed that the increase of the steam to biomass ratio leads to a decrease of the gasification temperature [34], as evidenced in Figure 10 for the two biomasses. This is due to the fact that the rise in water favors the formation of H_2 . The water gas shift reforming reaction (8) is exothermic, however, the steam–methane reforming reaction (10) is endothermic, with five times the enthalpy. In addition, as the steam enters at 100 °C, the reaction temperature is expected to diminish. In this way, the expected behavior that is observed is the reduction of the temperature with the upsurge of steam entering the reactor.

3.4. Effect of the Temperature of the Gasifier

The analysis of the influence of the gasification temperature on the molar composition and the heating value of the syngas was carried out with the gasification temperature as an independent variable, and with the composition of syngas, flow of syngas, and heating value as dependent variables. For this study, a biomass input of 5 kg/h is fixed. In addition, the gasification temperature was varied from 600 to 1200 °C, the air intake was fixed at 1.25 kg/h (approximately 0.4 ER) and there was no vapor inlet, so only the water present in the biomass moisture was used.



Figure 10. Effect of SBR on the temperature of the gasifier operated with hardwood chips (a) and almond shells (b).

3.4.1. Molar Composition of Syngas

The gasification temperature is another important parameter in the syngas production process. Hydrogen is expected to increase with the gasification temperature, reaching the maximum, and then gradually decrease at higher temperatures. Gasification is generally satisfactory at a temperature of 800 °C [12,27,33]. Figure 11 shows the behavior of the molar composition of the synthesis gas with the growth in the gasifier temperature for both biomasses. While CO increases, H₂ rises to a maximum and then declines with growing temperature. CO₂ and CH₄ decrease. This is due to the fact that the reactions of Boudouard (6), reforming char (7) and steam–methane reforming (10) are endothermic. Thus, with increasing temperature, the balance shifts to the formation of products, leading to the consumption of more CO_2 and CH_4 and to the production of more CO. The reactions of water gas shift reaction (8) and hydrogasification (9) are exothermic, so a higher temperature makes the reaction more difficult and the production of less CO₂, H₂, and CH₄. Hydrogen fluctuation can be caused by the combined effects of reactions in the gasification zone. The water gas shift reaction (8) is one of the most important for the final composition of the synthesis gas due to the ability to react with CO and H_2O and to form CO₂ and H_2 . At lower temperatures, the water gas shift reaction (8) prevailed in the production of H_2 , while at higher temperatures the action was impaired. The other two reactions for the formation of H_2 reforming char (7) and steam–methane reforming (10) are endothermic and may contribute to the increase. However, after the temperature of 800 $^{\circ}$ C, the reactions may be limited due to the lack of reagents such as CH₄ and H₂O. Thus, the combined effects of the reactions 7, 8, 9, and 10 can cause a reduction in hydrogen after 800 °C.



(a) hardwood chips

(**b**) almond shells

Figure 11. Effects of the gasifier temperature on the composition of syngas produced from hardwood chips (**a**) and almond shells (**b**).

3.4.2. Heating Value

The heating value tends to rise with increasing temperature in the gasifier since a surge in the composition of H_2 and CO in the synthesis gas is expected [17,34]. Figure 12 shows the behavior of the heating value when the temperature is varied for both biomasses. It is noticeable the rise in the heating value with the increase in the gasification temperature (approximately 4% for hardwood and 3% for almond shell). This is due to the fact that a growth in temperature favors the formation of H_2 and CO in the syngas, rising the calorific value. Even with the stabilization and slight decrease of hydrogen after the temperature of 800 °C, the CO continues to increase and a higher amount of CO in the syngas causes the energy released by the syngas to be higher, thus the growth of CO tends to augment the heating value.



Figure 12. Effect of the gasifier temperature on heating values of the synthesis gas obtained with hardwood chips (**a**) and almond shells (**b**).

3.5. Combined Effect of Equivalence Ratio and Steam to Biomass Ratio

The combined independent variables equivalence ratio and steam to biomass ratio were used to analyze the behavior of the composition of syngas, flow of syngas, and the gasification temperature, aiming to find maximum and minimum parameters of these independent variables in order to obtain a synthesis gas rich in CO and H₂. The air intake was varied up to 2.4 kg/h (approximately 0.8 ER), the feed of steam up to 3.6 kg/h (approximately 0.7 SBR), and the biomass intake remained fixed at 5 kg/h.

3.5.1. Carbon Monoxide

The previous analysis of ER and SBR showed that both the increase in air and in steam led to a decrease in the composition of CO in the syngas. Figure 13 shows how the combination of these two parameters influences the composition of carbon monoxide in the gas obtained at the end of the process for the two biomasses studied. As expected, the combined rise of ER and SBR reduces the composition in CO due to favoring the formation of H₂ and CO₂. It is necessary to analyze the other compositions to find the best combination of ER and SBR, however, it is observed that these values must be up to 0.5 (ER) and 0.2 (SBR), because combinations with values greater than these considerably decrease the composition of CO in the syngas.



(a) hardwood chips

(b) almond shells

Figure 13. Combined effects of ER and SBR on the composition of CO in the syngas produced with hardwood chips (**a**) and almond shells (**b**).

3.5.2. Hydrogen

The previous ER study showed that the increase in air first increases the amount of H_2 and after values of 0.4 and 0.5 (for hardwood chips and almond shells, respectively) that amount decreases. The SBR analysis showed that the increase of steam feed favors the composition of H_2 in the syngas. Figure 14 shows how the combination of these two parameters affects the composition of H_2 for both biomasses. It is observed that the increase of ER up to 0.4 (in Figure 14a) and 0.5 (in Figure 14b) causes the composition of H_2 to grow, decreasing after that value. The upsurge in steam favors the formation of H_2 , obtaining compositions higher than 50%. It is observed that the best values to obtain a syngas rich in H_2 is with ER between 0.3 and 0.5 because the lack of air or the excess causes a decline in H_2 . The feed of steam favors the formation of H_2 , but it also favors the formation of CO_2 and decreases the composition of CO. Therefore, it is necessary to analyze the composition of CO_2 to choose the best SBR input parameter.



(a) hardwood chips

(**b**) almond shells

Figure 14. Combined effects of ER and SBR on the composition of H_2 in the syngas produced with hardwood chips (**a**) and almond shells (**b**).

3.5.3. Carbon Dioxide

From the previous ER and SBR analyzes, it can be observed that the increase of both air and steam favor the formation of CO_2 . Figure 15 shows the behavior of the CO_2 composition in the synthesis gas when these two parameters are combined. It is observed that larger ER and SBR values lead to higher amounts of CO_2 in the syngas. Therefore, the best range for working with air and steam is up to 0.5 for ER and 0.2 for SBR.





Figure 15. Combined effects of ER and SBR on the composition of CO₂ in the syngas produced with hardwood chips (**a**) and almond shells (**b**).

3.5.4. Molar and Mass Flow of Syngas

The previous ER study showed that the increase of air first increases the molar flow of syngas and that after 0.4 and 0.5 (for hardwood chips and almond shell, respectively) the flow decreases. Regarding the mass flow, there is a rise in value, regardless of the ER. The analysis of the SBR effect showed that the increase in steam favors the molar and mass flows. Figure 16 shows how the combination of these two parameters interferes in the molar and mass production of syngas for both biomasses. It is observed that the increase of ER up to 0.4 for hardwood chips and 0.5 for almond shells, causes the molar flow to increase, decreasing after that value. The upsurge in steam favors the molar production of syngas. Note that the best values for higher molar flow occur between 0.3 and 0.5 due to the fact that the lack of air or the excess causes the amount of H₂ to decline and consequently the molar flow as well. The feeding of steam favors the molar production of syngas. However, the growth in SBR, in addition to increasing the composition of H₂, increases the composition of CO₂.





Figure 16. Combined effects of ER and SBR on the molar and mass flow of syngas produced with hardwood chips (**a**) and almond shells (**b**).

It is also observed that the increase of both ER and SBR rises the mass flow of syngas. As observed in the molar flows, after ER values of 0.4 and 0.5 (hardwood chips and almond shells, respectively) there is a decrease in the molar flow caused by the decline of H₂ and the increase in SBR favors the composition of H₂, but also increases the composition of CO₂. Thus, although the ER and SBR increase the mass flow of syngas, this flow may not have the best compositions of H₂ and CO. Therefore, in relation to the production of syngas, it is recommended to work with ER values between 0.3 and 0.5 and low SBR.

3.5.5. Temperature of the Gasifier

The analysis of the SBR influence showed that the growth in steam decreases the temperature of gasification. The previous ER study showed that the increase in air initially lowers the gasification temperature and that after 0.4 (for hardwood chips) and 0.45 (for almond shells) the temperature starts to rise. Figure 17 shows the combined influence of these two parameters in the reaction temperature for both biomasses. The decreasing temperature with increasing steam was evident with any value of ER. However, it should be noted that the behavior of decreasing the temperature and then rising when the ER is increased does not happen in all steam input values. It can be observed that from the steam to biomass ratio of 0.1, the gasification temperature does not decrease and then increases with the variation of the air intake. A rise in the temperature only occurs with the surge of ER. This can be explained by the fact that the steam input ends up favoring more than the others the formation reactions of H_2 water gas shift reaction (8) and steammethane reforming (10). And as steam–methane reforming is endothermic with an enthalpy five times greater than the water gas shift reaction, the tendency is for the gasification temperature to reduce. However, as of the input of 0.1 SBR, only the water gas shift reaction is favored because the CH_4 that was available was consumed. Therefore, there will be a greater release of energy than consumption. Thus, from 0.1 to steam to biomass ratio, the temperature tends to only rise with the increase of ER.



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Figure 17. Combined effects of ER and SBR on the temperature of the gasifier operated with hardwood chips (**a**) and almond shells (**b**).

Thus, with the analysis of the influence of the variation of ER and SBR in the composition of syngas for CO, H_2 , CO_2 , and CH_4 , it can be inferred that a combination of ER between 0.3 and 0.5 and SBR up to 0.2 is the range in which the best CO and H_2 compositions are obtained, with small amounts of CO_2 and CH_4 . These compositions are obtained at temperatures between 850 and 950 °C.

4. Conclusions

In this work, a downdraft gasifier was modeled and simulated for two residual biomasses (forest and agricultural) in order to predict the composition of the syngas produced. The reactors simulated gasification by minimizing the free energy of Gibbs. The main operating parameters were the equivalence ratio, steam to biomass ratio, and gasification temperature. In the simulations, a sensitivity analysis was carried out, where the effects of these parameters on the composition of syngas, flow of syngas, and heating values were studied.

The model is able to predict the gasifier's performance and is qualified to analyze the behavior of the independent parameters in the gasification results. The following are the main results achieved with the simulation:

- The mass flow of syngas is favored by the increase of ER and SBR;
- The molar flow upsurges with higher SBR, however, it reaches a maximum value with rising ER;
- The heating value of the syngas declines with increasing ER and SBR, but increases with the growth of gasification temperature;
- The composition of H₂ and CO₂ improves with SBR increase, while CO declines continuously;
- An SBR value up to 0.2 is an acceptable value to promote the production of H₂ without so much formation of CO₂ in the syngas;
- The equivalence ratio is a key parameter in the process as it favors the production of H₂. A low amount causes the absence of gasification and a high amount causes formation of CO₂, decrease of CO, and the presence of N₂ in the synthesis gas;
- An ER value between 0.3 and 0.5 is within the favorable range to maximize the amount of CO and H₂ in the process;
- The favorable temperature of the gasifier must be between 850 and 950 °C, controlling the feeds of air and steam to obtain these values.

Additionally, it is concluded that in the specific conditions where the gasification temperature is specified and changed for a fixed air intake, the content of CO tends to rise

with increasing temperature, but the content of H_2 reaches a maximum for an optimal temperature value, while CO_2 and CH_4 tend to decrease continuously.

In summary, with a temperature between 850 and 950 °C, SBR values up to 0.2 and ER values between 0.3 and 0.5, the best operating conditions are obtained to maximize the composition of the syngas rich in CO and H_2 .

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