Modeling and simulation of biomass gasification processes

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Abstract

Biomass gasification is the conversion of organic materials into an energetic gas, rich in hydrogen and carbon monoxide, 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 provides an analysis of the process performance, allowing for resources 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, applying the tools available in the simulator database in order to satisfactorily reproduce a downdraft gasifier operation behavior. The study was done for two residual biomasses (forest and agricultural) in order to predict the produced syngas composition. The reactors simulated gasification by minimizing Gibbs free energy. The main operating parameters were the equivalence ratio, steam to biomass ratio and gasification temperature (independent variables). In the simulations, a sensitivity analysis was carried out, where the effects of these parameters on the syngas composition, syngas flow 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 gasifier's performance and is qualified to analyze the behavior of the independent parameters in the gasification results. In summary, with a temperature between 850 and 950°C, SBR up to 0,2 and ER between 0,3 to 0,5, the best operating conditions are obtained for maximize the composition of the syngas rich in CO and H_2.

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

Resumo

A gaseificação de biomassa é a conversão de materiais orgânicos em um gás energético, rico em hidrogênio e monóxido de carbono, através de reações de oxidação e redução a temperaturas elevadas. Na avaliação dos processos de gaseificação, estimar a composição do gás combustível para diferentes condições é fundamental para identificar as melhores condições de operação. Dessa forma, a modelagem e simulação de gaseificação fornecem uma análise do desempenho do processo, permitindo economias de tempo e recursos na operação do processo em escala piloto, pois possibilitam uma previsão do comportamento e uma análise dos efeitos de diferentes variáveis no processo. Assim, o foco deste trabalho foi a modelagem e simulação de processos de gaseificação de biomassa usando o software de processos químicos UniSim Design, aplicando as ferramentas disponíveis no banco de dados do simulador, a fim de reproduzir satisfatoriamente o comportamento de uma operação de um gaseificador de fluxo descendente. O estudo foi realizado para duas biomassas residuais (florestal e agrícola), a fim de prever a composição do syngas. Os reatores simularam a gaseificação, minimizando a energia livre de Gibbs. Os principais parâmetros operacionais foram a razão de equivalência, relação vapor/biomassa e temperatura de gaseificação (variáveis independentes). Nas simulações, foi realizada uma análise de sensibilidade, onde foram estudados os efeitos desses parâmetros na composição do syngas, fluxo do syngas e valor de aquecimento (variáveis dependentes), com o intuito de maximizar essas três variáveis no processo com a escolha dos melhores parâmetros de operação. O modelo é capaz de prever o desempenho do gaseificador e está qualificado para analisar o comportamento dos parâmetros independentes nos resultados da gaseificação. Em resumo, com uma temperatura entre 850 e 950°C, SBR até 0,2 e ER entre 0,3 e 0,5, são obtidas as melhores condições de operação para uma maximização da composição do syngas rico em CO e H_2.

Palavras-chave: gaseificação de biomassa; gaseificador de fluxo descendente; simulação de processo; UniSim Design.

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LIST OF ACRONYMS

BFB	Bubbling fluidized bed gasifier
CFB	Circulating fluidized bed gasifier
ER	Equivalence ratio
FC	Fixed carbon
MSW	Municipal Solid Waste
N	Normal (1atm, 0°C)
SBM	Simulation Basis Manager
SBR	Steam to biomass ratio
VM	Volatile matter

Chapter 1 – Introduction

1.1 MOTIVATION AND OBJECTIVES

Fossil fuel is still the main source of energy used worldwide, due to its high energy efficiency. However, in addition to the pollution caused by the released gases, the fossil energy is finite, being currently depleting fast, boosting the search and the need to use renewable energies (Keche et al, 2015). Under this context, solid biomass shows great potential to become an energetic alternative of fossil energy sources. This renewable energy is abundant and has a virtually zero carbon dioxide (CO_2) balance, since the CO_2 produced in power generation is equivalent to the CO_2 consumed during the growth of the plant from which the biomass originated (Tavares et al., 2020).

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 (Tavares et al., 2020). The amount of forest waste in Portugal is approximately 2,2 million tons per year. Besides, 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 (Lourenço et al, 2012; Tavares et al, 2020; ICNF, 2014).

One system to generate energy from biomass is gasification. This process is not new, it was developed during the nineteen and twenty centuries, mainly for coal. However, recently, biomass gasification has been studied and seen as an energy alternative since, besides generating clean energy, it provides a destination for wastes that would be otherwise discarded (Silva et al, 2014).

Biomass gasification is the conversion of organic materials into an energetic gas, rich in hydrogen (H_2) and carbon monoxide (CO), through oxidation and reduction reactions at elevated temperatures. This conversion can be performed in various types of reactors, such as fixed and fluidized bed. 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 provides a previous virtual analysis of the process performance, allowing for resources and time savings in pilot-scale process operation, as it predicts the behavior and analyzes the effects of different variables on the process (McKendry, 2002c; Mansaray et al, 2000).

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 a gasifier operation behavior. 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).

1.2 LAYOUT

In order to complete these objectives, the work was divided into a few chapters. The first chapter (Chapter 1 - Introduction) presents an introduction to the framework of the studied issue and explains the relevance of the proposed simulation work, containing the motivation, objectives and the layout of the report; the second chapter (Chapter 2 - State of the Art) presents the bibliographic review with the most important information collected from the literature; the third chapter (Chapter 3 - Model Development) shows in detail the modeling procedure developed in order to simulate a biomass gasification process; the fourth chapter (Chapter 4 - Results and Discussion) presents all the results obtained from the simulations carried out and the correspondent discussion; finally, the fifth chapter (Chapter 5 - Conclusions and Future Works) includes relevant conclusions obtained from the accomplishment of this work, and the proposal of possible ideas for future works and lines of research.

Chapter 2 – State of the art

2.1 BIOMASS

Biomass is any material derived from plants or waste with potential energy for the production of electricity, heat or fuels. This organic matter, rich in carbon (C), oxygen (O), nitrogen (N) and hydrogen (H), can be aquatic, as algae or terrestrial as wood, urban, industrial or agricultural solid wastes. Biomass is the biodegradable fraction of these wastes that allows the generation of energy through thermal, chemical and biochemical processes (Brás et al, 2012). Biomass absorbs CO_2 from the atmosphere during photosynthesis and CO_2 is returned to the environment after combustion. Because of this, biomass is CO_2 neutral, making it a sustainable and advantageous fuel to replace fossil fuels as concerns about global warming increase (Tavares et al, 2020).

2.1.1 TYPES OF BIOMASS

Biomass can be classified in two groups: waste and virgin biomass. These two groups can further be divided into 6 categories, as shown in Table 1.

Table 1. Major groups of biomass and their sub classification (Bhavanan and Sastry, 2011).

Virgin	Terrestrial biomass	Forest biomass, grasses, energy crops, cultivated crops
	Aquatic biomass	Algae, water plant
Waste	Municipal waste	Municipal solid waste biosolids, sewage, landfill
	Agricultural solid waste	Livestock and manures, agricultural crop residue
	Forestry residues	Bark, leaves, floor residues
	Industrial wastes	Black liquor, demolition wood, waste oil or fat

The biomass of the virgin biomass group is cultivated for energy production. Examples include eucalyptus, willows, poplars, assorghum, sugar cane, soya beans, sunflowers and cotton. These energy crops are suitable for use in combustion, pyrolysis and gasification process, for the production of biofuels, synthesis gas (syngas) and hydrogen (Bhavanan and Sastry, 2011; Lasa et al, 2011).

In the waste biomass group, agricultural waste is generated in a large volume. The most common is rice husk, which represents 25% of rice by mass. Other plant residues include sugarcane fiber, coconut husks and shells, groundnut (peanut) shells and straw. Animal manure (such as cattle, chicken and pork) is also included in the agricultural waste examples. However, due to the low heating value of the syngas produced from animal manure, this residue is not technically viable as a gasifier fuel. A possibility may consider the use of another biomass as a supplement to mix it with animal manure. Another type of waste biomass is forest waste, such as mill wood, tree and shrub waste.

Finally, municipal and industrial waste are other types of biomass within the waste group. Examples are Municipal Solid Waste (MSW), sewage sludge and industry waste, such as black liquor from wood pulping. They have great potential as raw material, but present problems in the gasification process, since they form a large amount of ash deposits in the furnace or inside the boiler convective sections (Lasa et al, 2011).

2.1.2 COMPONENTS OF BIOMASS

The main components of biomass are varying amounts of cellulose, hemicellulose and lignin. Cellulose is a long chain glucose polymer and is a major constituent of the plant cell walls. Hemicellulose is a mixture of polysaccharides including glucose, xylose and uranic acids, which can be linear or branched. Lignin can be considered as a high molecular weight amorphous group. It has the function of ensuring rigidity and resistance to the cell wall. Woody species are characterized by slow growth and composed of tightly bound fibers, giving a hard surface, while herbaceous species have more loosely bound fibers, indicating a lower proportion of lignin. The ratio between cellulose and lignin is a determining factor in identifying the energy power of biomass. Since the biodegradability of cellulose is higher than that of lignin, biomass containing a higher proportion of cellulose to lignin provides a higher energy yield in processes that use biomass as raw material (Bhavanan and Sastry, 2011; McKendry, 2002a). Table 2 shows some types of biomass and the respective typical percentages of cellulose, hemicellulose and lignin.

Table 2. Lignin, cellulose and hemicellulose content of different types of biomass (Bhavanan and Sastry, 2011).

Plant	**Lignin (wt. %)**	**Cellulose (wt. %)**	**Hemicellulose (wt. %)**	**Ash (wt. %)**
Subabul wood	24,7	39,8	24,0	0,9
Wheat straw	16,4	30,5	28,9	11,2
Bagasse	18,3	41,3	22,6	2,9
Corn cob	16,6	40,3	28,7	2,8
Groundnut shell	30,2	35,7	18,7	5,9
Coconut shell	28,7	36,3	25,1	0,7
Millet husk	14,0	33,3	26,9	18,1
Rice husk	14,3	31,3	24,3	23,5

2.1.3 COMPOSITION OF BIOMASS

There are two main composition analyzes for solid fuels: the approximate and the ultimate analysis. The first analysis is based on chemical energy stored in two forms: fixed and volatile carbons. The volatile matter (VM) of a fuel is that part taken as gas (including moisture) upon heating (at 950°C for 7 min under inert atmosphere). The fixed carbon (FC) content is the mass that remains in the sample after the release of volatiles, excluding ash and moisture. This analysis provides a measure of how easily biomass can be ignited and subsequently gasified or oxidized, where the higher is the fixed carbon content the higher is the energetic potential.

The ultimate analysis allows the quantification of the main elements present in biomass: carbon, hydrogen and oxygen, as well as other elements such as nitrogen and sulfur (S). This is a more expensive analysis compared to the approximate analysis, but it presents a more detailed diagnosis of all elements present in the studied biomass (McKendry, 2002a).

The approximate analysis of some biomass sources is presented in Table 3 and the respective ultimate analysis is shown in Table 4.

Table 3. Approximate analysis of different biomass sources.

Biomass	**Moisture (%)**	**VM (%)**	**FC (%)**	**Ash (%)**	
Grass	0,0	79,7	15,0	5,3	Smeenk and Brown, 1998
Rice husk	11,7	53,1	20,4	14,8	Yin et al, 2002
Bituminous coal	11,0	35,0	45,0	9,0	McKendry, 2002
Wheat straw	16,0	59,0	21,0	4,0	McKendry, 2002
Barley straw	30,0	46,0	18,0	6,0	McKendry, 2002
Coal	2,6	41,8	54,1	1,5	Ocampo et al, 2003
Sugarcane bagasse	5,9	74,0	13,2	6,9	Castro et al, 2009
Forest residues	11,3	70,8	17,7	0,2	Silva et al, 2014
Coffee bark	25,3	62,1	10,7	1,9	Silva et al, 2014
Vine pruning waste	13,3	72,5	11,5	2,7	Silva et al, 2014
Food waste	29,4	51,1	14,6	4,9	Ramzan et al, 2011
Urban solid waste	50,9	18,8	7,6	22,7	Ramzan et al, 2011
Poultry waste	7,5	40,3	8,4	43,8	Ramzan et al, 2011
Solid waste	46,81	32,05	9,84	11,3	Araújo, 2016

Table 4. Ultimate analysis of different biomass sources.

Biomass	**C**	**H**	**O**	**N**	**S**	**Ash**	
Grass	46,8	5,1	42,1	0,6	0,1	5,3	Smeenk and Brown, 1998
Rice husk	36,7	5,5	42,5	0,3	0,5	14,5	Yin et al, 2002
Bituminous coal	73,5	5,5	8,8	1,4	1,7	9,1	McKendry, 2002
Wheat straw	49,8	5,7	40,0	0,3	0,1	4,1	McKendry, 2002
Barley straw	47,3	6,3	39,7	0,4	0,1	6,2	McKendry, 2002
Coal	75,3	5,4	15,6	1,8	0,4	1,5	Ocampo et al, 2003
Sugarcane bagasse	45,2	5,4	41,8	0,2	0,02	7,4	Castro et al, 2009
Forest residues	43,0	5,0	49,6	2,4	-	-	Silva et al, 2014
Coffee bark	40,1	5,6	49,1	5,2	-	-	Silva et al, 2014
Vine pruning waste	41,3	5,5	50,6	2,6	-	-	Silva et al, 2014
Food waste	56,7	8,8	23,5	3,9	0,2	6,9	Ramzan et al, 2011
Urban solid waste	36,4	5,0	10,1	1,4	0,8	46,3	Ramzan et al, 2011
Poultry waste	22,4	3,8	27,1	2,6	0,7	43,4	Ramzan et al, 2011
Solid waste	47,9	6,3	33,3	1,0	0,2	11,3	Araújo, 2016

2.1.4 BIOMASS CONVERSION PROCESSES

There are many possible conversion routes to produce energy products from biomass. The flowcharts in Figures 1 and 2 illustrate the main conversion routes used or under development for the production of heat, energy and transportation fuels. There are three main technologies: thermochemical, biochemical and physicochemical. For thermochemical conversion, the main processes are combustion, gasification, pyrolysis and liquefaction. For biochemical conversions, the most common routes are anaerobic digestion, for the production of biogas, and fermentation, for the synthesis of bioalcohols, mainly bioethanol. For the physicochemical process, the main process is lipid extraction with the subsequent production of biodiesel (McKendry, 2002b; Faaij, 2006; Goyal, 2008).

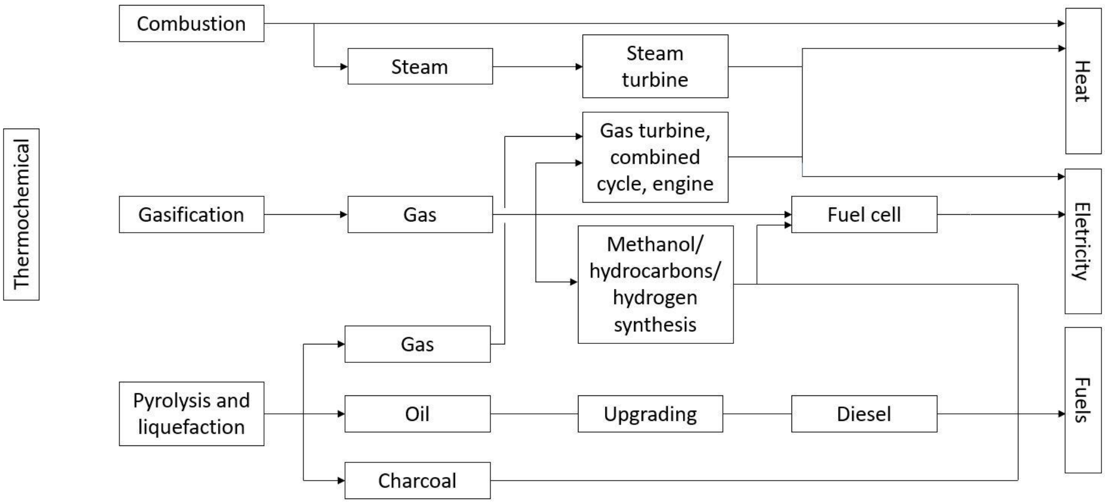


Figure 1. Main processes, intermediate energy carriers and final energy products from thermochemical conversion of biomass (Faaij, 2006).

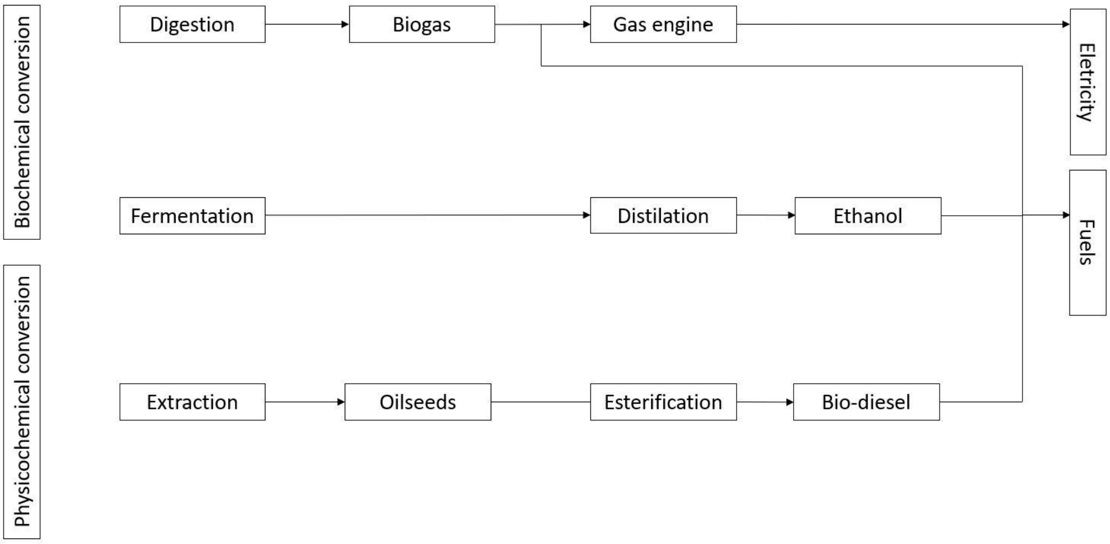


Figure 2. Main processes, intermediate energy carriers and final energy products from biochemical and physicochemical conversion of biomass (Faaij, 2006).

2.2 GASIFICATION OF BIOMASS

Gasification is the conversion of biomass into a combustible gas, by heating biomass in a gasification medium such as oxygen (O_2), steam or air. This gas is a gaseous mixture composed mainly of carbon monoxide (CO), hydrogen (H_2) and methane (CH_4). 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 (McKendry, 2002b). 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 oxidant amount, feedstock composition, gasifier temperature and reactor geometry (Patra and Sheth, 2015; Bach et al, 2019).

The process of biomass gasification involves reactions related to various phenomena such as drying (endothermic), pyrolysis (endothermic), oxidation (exothermic) and reduction (endothermic). In the drying phase, the moisture content of the biomass is reduced to less than 5%, occurring at temperatures of 100-200°C. In general, the moisture content of biomasses varies between 5-35wt.%. In the pyrolysis phase occurs the thermal decomposition of biomass, in the absence of oxygen or air, and volatile matter is released due to the thermal breakdown of biomass. As a result, gas mixtures containing oxygen, hydrogen, nitrogen and hydrocarbons are released and the biomass is reduced to solid coal. Hydrocarbon gases condense at low temperatures and generate liquid tars. Gases released from the drying and pyrolysis zones may or may not pass through the oxidation zone, depending on the type of gasifier.

Combustion is a reaction between carbonized solid biomass and oxygen, resulting in the formation of CO_2. Hydrogen present in biomass is also oxidized to generate water (H_2O). The excessive heat released from carbon and hydrogen oxidation is used for drying, pyrolysis and gasification reactions. In gasification, various reduction reactions take place at temperatures ranging between 800 and 900°C. These reactions are mainly endothermic in nature (Patra and Sheth, 2015; Molino et al, 2018).

The main gasification reactions are shown in Table 5 (Castro et al, 2009; Patra and Sheth, 2015; Ramzan et al, 2011; Bassyouni et al, 2014; Fabry et al, 2013; Molino et al, 2018).

Table 5. Main reactions involved in gasification processes.

Gasification Step	**Reaction**		**ΔH° (kJ.mol^{-1})**
Pyrolysis	Biomass → Char +Tar +Volatiles (1)		
Oxidation	$Char(s) + O_2 \rightarrow CO_2$	Carbon Oxidation (2)	-394
	$C(s) + 0{,}5O_2 \rightarrow CO$	Carbon Partial Oxidation (3)	-110
	$CO + 0{,}5O_2 \rightarrow CO_2$	Carbon Monoxide Oxidation (4)	-283
	$H_2 + 0{,}5O_2 \rightarrow H_2O$	Hydrogen Oxidation (5)	-242
Reduction	$C(s) + CO_2 \leftrightarrow 2CO$	Boudouard Reaction (6)	172
	$C(s) + H_2O \leftrightarrow CO + H_2$	Reforming of Char (7)	131
	$CO + H_2O \leftrightarrow CO_2 + H_2$	Water Gas Shift Reaction (8)	-42
	$C(s) + 2H_2 \leftrightarrow CH_4$	Hydrogasification (9)	-75
	$CH_4 + H_2O \leftrightarrow CO + 3H_2$	Steam-methane Reforming (10)	206

- Step (1) is also called devolatilization, where volatiles are released.
- Reaction (2) is the complete combustion of carbon (exothermic reaction).
- Reaction (3) is incomplete carbon combustion (exothermic reaction).
- Reaction (4) is CO oxidation (exothermic reaction).
- Reaction (5) is H_2 oxidation (exothermic reaction).
- Reaction (6) is a process that produces CO (endothermic reaction).
- Reaction (7) is a heterogeneous shift reaction (endothermic reaction).
- Reaction (8) is a gas-water displacement reaction (exothermic reaction).
- Reaction (9) is a hydrogenation reaction (exothermic reaction).
- Reaction (10) is the methane reforming reaction (endothermic reaction).

2.2.1 DESIGN OF GASIFIER

The gasifier is the reactor where the chemical conversion of the carbonaceous material occurs. The two main types of gasifier are fixed bed and fluidized bed. A third type was developed with dragging suspension, but the feed needs to be finely divided, being infeasible for fibrous materials, such as wood, thus making the process unsuitable for most of the biomasses. The two basic configurations, according to the reaction bed arrangement, vary with the type of biomass used, the way the oxidizing agent is introduced into the reactor and the temperatures and pressures considered. Fixed bed gasifiers are divided between co-current and countercurrent bed and fluidized bed gasifiers between bubbling and circulating bed, as shown in Figure 3. Fixed bed reactors are mainly used for small scale production. On the other hand, in the fluidized bed reactors, bubbling bed reactors are recommended for medium scale production and circulating bed reactors for industrial scale processes. These 4 variations represent over

95% of the gasifier configurations, with less than 5% intended for variants of the two main models (Maniatis, 2001; McKendry, 2002c; Molino et al, 2016).

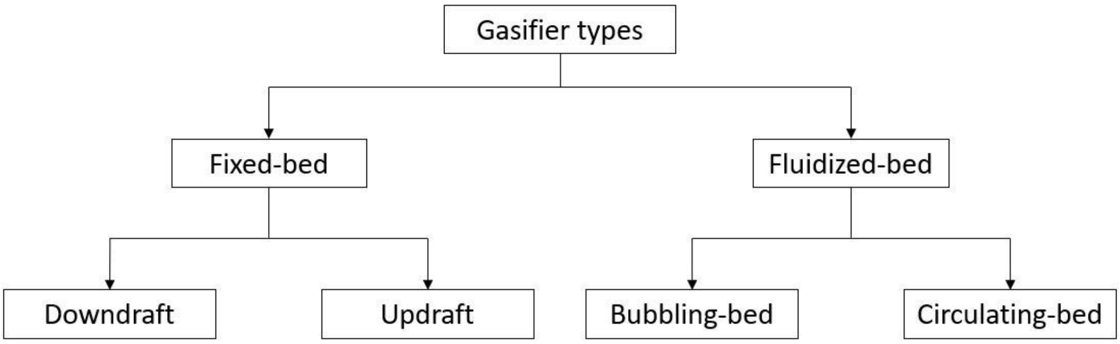


Figure 3. Main gasifier types.

2.2.1.1 FIXED-BED GASIFIERS

Fixed bed gasifiers are characterized by a bed formed by feedstock (biomass) that slowly descends by the action of gravity while it is converted into gaseous products. Since the charge is made from the top of the reactor, the direction of the gas flow in relation to the charge movement defines the two main variations: updraft and downdraft. This type of gasifier is relatively easy to design and operate compared to the fluidizing gasifier (Rodrigues, 2015; Carvalho, 2012; Molino et al, 2016).

2.2.1.1.1 UPDRAFT GASIFIER

In the updraft gasifier design (see Figure 4), the solid material is inserted in the top and the oxidizing gas is introduced in the bottom of the reactor. There is a grid at the bottom of the reactor that prevents the entrance of the gasifying agent from being blocked, also acting as support of the reactor bed. In this way, the solid material is converted to combustible gas as it moves to the bottom of the reactor. The reactions start at the bottom of the reactor with biomass combustion. After combustion begin, water vapor and carbon dioxide are released from the feedstock. These gases, generated with temperatures above 1000°C, begin to rise, passing to the area where the reduction reactions occur, producing hydrogen and carbon monoxide, thus removing energy from the system and consequently reducing the temperature.

The gases produced in the combustion and reduction zones give rise to an environment of total oxygen absence, creating the pyrolysis zone. Finally, the drying zone uses the remaining heat from the gas to dry the biomass entering the reactor. The synthesis gas is withdrawn from the reactor from the top, leaving at temperatures between 200-300°C, therefore having a medium/high energy efficiency. Due to its characteristics, this gasifier design leads to high concentration of tar in the generated gas, so it is advisable to apply it for thermal purposes. If it is intended to be applied to an engine, gas cleaning is required, making the process more complex (Carvalho, 2012; Balat, 2009; Panwar et al, 2012).

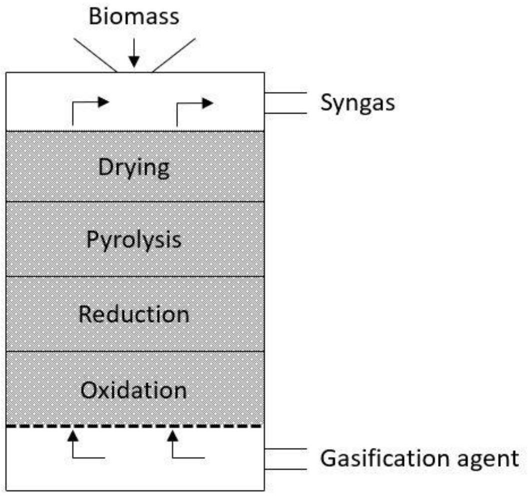


Figure 4. Updraft gasifier.

2.2.1.1.2 DOWNDRAFT GASIFIER

The downdraft gasifier design (see Figure 5) 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 flowing into the reduction zone and 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°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 is limited in scale. It also needs specific biomass conditions and is not suitable for various types of biomass (McKendry, 2002c; Patra and Sheth, 2015).

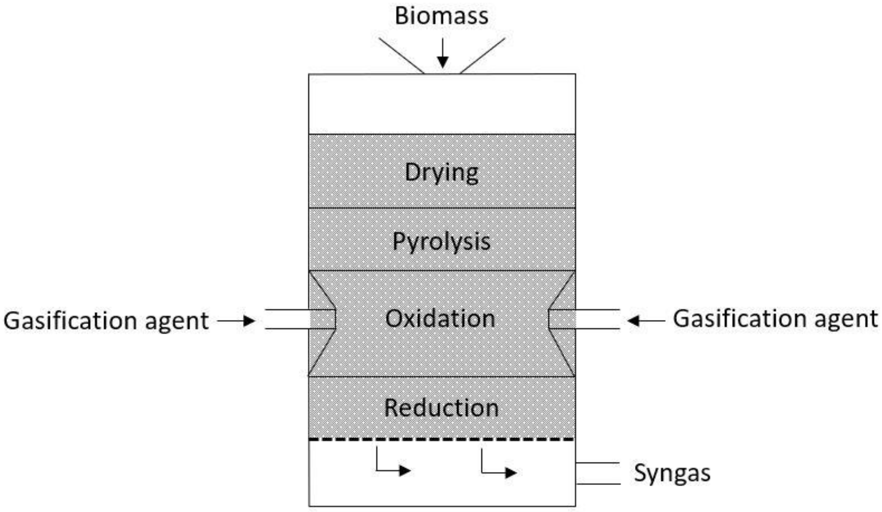


Figure 5. Downdraft gasifier.

2.2.1.2 FLUIDIZED BED GASIFIERS

Among gasification technologies, fluidized beds have greater fuel flexibility and high efficiency. However, the system is more sophisticated when compared to the fixed bed system. It is a reactor that can maintain uniform bed temperature, ensuring a more effective mix between the gasifying agent and the solid material, due to the way this gas is introduced into the reactor. In this reactor there are no different reaction zones. Biomass is introduced into the reactor and rapidly mixed with the bed and heated almost instantaneously to the bed temperature. Due to the quickness of the temperature rise, pyrolysis occurs rapidly, resulting in a mixture of generated gases and solid components. In this type of gasifier, the cleaning of the gas is necessary due to the dragging of the ashes. The main difference between the two types of fluidized gasifiers is the rate at which the gasifying agent enters the reactor. While the bubbling fluidized bed gasifier (BFB) operates at low speeds, less than pneumatic transport, the circulating fluidized bed gasifier (CFB) operates at higher speeds, close to the pneumatic transport regime. (Rodrigues, 2015; Patra and Sheth, 2015; Panwar et al, 2012).

2.2.1.2.1 BUBBLING FLUIDIZED BED GASIFIER

The bubbling fluidized bed gasifier (see Figure 6) is flexible with respect to the type of biomass used. This gasifier allows a large heat transfer between the bed and the gasifying fuel. The gasifying agent is fed from the bottom of the reactor and the biomass is introduced above the grid. Temperature regulation is made by controlling the ratio of gasifying agent/biomass. Due to the high degree of mixing between the solid and partially gassed particles, there may be particles that leave the bed still containing unconverted carbon due to the low residence time in the reactor. One issue to note is the slow diffusion of oxygen from the bubbles in the dense region. As a consequence, in the gas phase, oxidation reactions are predominant over reduction, decreasing process efficiency (McKendry, 2002c; Carvalho, 2012; Molino et al, 2016).

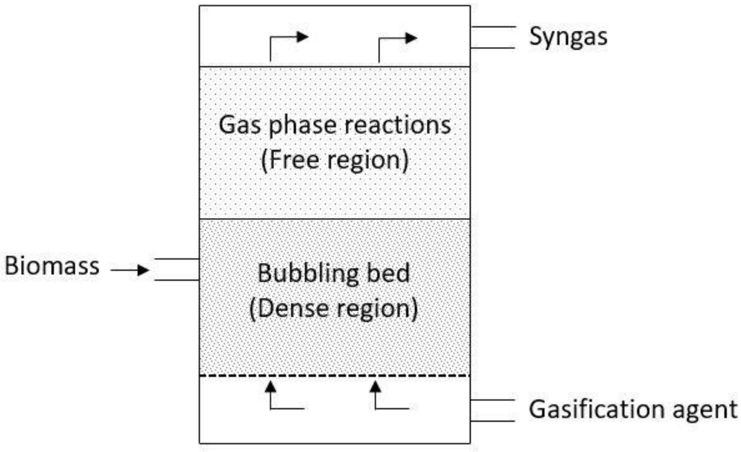


Figure 6. Bubbling fluidized bed gasifier.

2.2.1.2.2 CIRCULATING FLUIDIZED BED GASIFIER

Gasification using circulating fluidized bed systems (see Figure 7) at high fluidization velocity generates a turbulent regime, thus there is no well-defined separation between the zone of dense and diluted solids, as occurs in the bubbling beds. Hence, bed particles are dragged out of the reactor and it is necessary to recycle these solids, separating them from the gas through a cyclone, and then returning the solids to the bed. This particle recirculation provides high carbon conversion by increasing the residence time of solid particles within the reactor, thereby improving the quality of the synthesis gas. This gasifier can operate at higher pressures. For large scale production it is the most recommended gasifier (Balat, 2009; Molino et al, 2016).

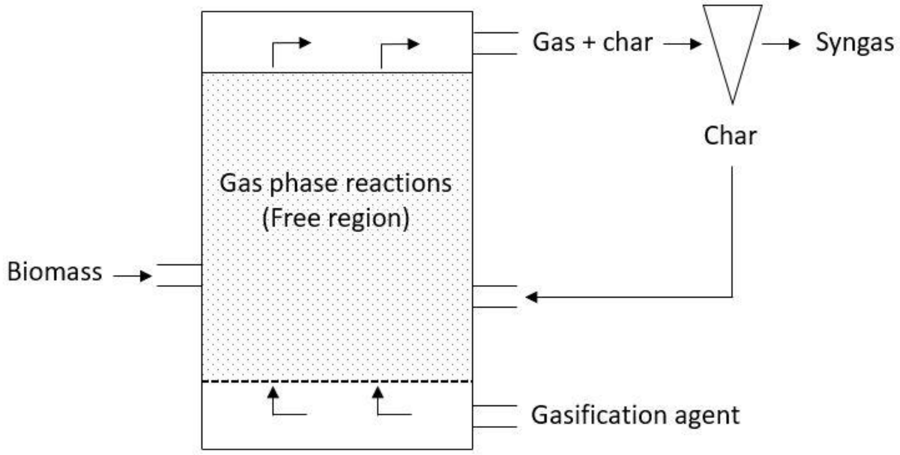


Figure 7. Circulating fluidized bed gasifier.

2.2.1.3 ADVANTAGES/DISADVANTAGES OF THE TYPES OF GASIFIERS

The selection of the gasifier type and design depends on various factors such as material properties, the required gas quality, heating method and operating conditions. Therefore, the main criteria for choosing a reactor are capital costs, operation, maintenance, robustness of the gasifier configuration and prior preparation of the raw material.

Fluidized bed gasifiers need a more developed technology due to design and operation complexities. However, for large scale operations, they are the best suited for process flexibility, temperature uniformity and material diversity. As disadvantages, the high investments and maintenance costs required. Besides, it requires reduced particle sizes in the feed and pre-treatment processing such as drying, separation and downsizing. The size reduction needed can produce very fine solids that are not suitable for fluidization.

For small-scale gasification, focused on low calorific gas, fixed bed gasifiers are the most suitable, due to their simple design, simpler maintenance and no need for many prior raw material treatments. In Table 6 are listed the main advantages and disadvantages of each type of gasifier (Warnecke, 2000; McKendry, 2002c; Patra and Sheth, 2015; Molino et al, 2016).

Table 6. Advantages and disadvantages of different gasifier types (McKendry, 2002; Molino et al, 2016).

Reactor type	**Advantages**	**Disadvantages**
Fixed bed, updraft	Simple, inexpensive process Exit gas temperature about 250°C High carbon conversion efficiency Low dust levels in gas High thermal efficiency Can handle different materials Can handle materials with high moisture	Large tar production Potential channeling Potential bridging Small feed size Potential clinkering
Fixed bed, downdraft	Simple process Only traces of tar in product gas High carbon conversion efficiency	Minimum feed size Limited ash content allowable in feed Limits to scale up capacity Potential for bridging and clinkering High exit gas temperature Low thermal efficiency Requires materials with a low moisture content
Bubbling fluidized bed	High mixing and gas-solid contact High carbon conversion Good temperature control Can handle materials with different characteristics	Loss of carbon in the ashes Dragging of dust and ashes Restrictions on the size Relatively low process temperature to avoid phenomena of bed fluidization High investment and maintenance costs
Circulating fluidized bed	Flexible process Lower tar production High carbon conversion Good ability to scale-up Able to pressurize High volumetric capacity High CH_4 in product gas	Corrosion and attrition problems Possibility of casting the ashes Loss of carbon in the ashes High product gas temperature Restricted solid-gas contact Need for special materials Complex technology and difficult control Security issues High start-up and investment costs Requires the reduction of particle size and preparation supply

2.2.2 GASIFICATION CONDITIONS

Carbon conversion, product gas composition, formation and tar reduction are important indicators for biomass gasification. The parameters that affect these indicators are mainly temperature, pressure, moisture, gasifying agent, residence time, equivalence ratio and steam to biomass ratio.

2.2.2.1 TEMPERATURE

A gasification operating temperature greater than 800°C in the gasifier is recommended to avoid high tar formation. As the temperature increases, the content of the fuel gas, gas yield, hydrogen and heating value increase, while the tar content decreases. Therefore, the temperature has a favorable range. Rising the temperatures to values above 1000°C ash melting will occur, being thus not recommended for the process. The ideal temperature range for gasification is between 800 and 900°C (Skoulou et al, 2009; Lasa et al, 2011).

2.2.2.2 PRESSURE

As the pressure on the gasification process increases, the tar content decreases. However, higher pressures require higher technology and higher investment in the construction and maintenance of the gasifier. Small-scale gasifiers are usually operated at atmospheric pressure (Lasa et al, 2011; Molino et al, 2018).

2.2.2.3 MOISTURE

Moisture in the feed material affects the composition of the fuel gas, since very high humidity generates gas with low calorific value. Conversion efficiency decreases with increasing humidity, due to the large amount of energy consumed in water vaporization, which subsequently reduces the temperature of the gas. Limitations of biomass moisture content also depend on the type of gasifier, affecting mainly the fixed bed reactors. While in the updraft gasifier the humidity value can be high, in the downdraft gasifier this value cannot exceed 40% on dry basis (Bhavanam and Sastry, 2011; Lasa et al 2011).

2.2.2.4 GASIFYING AGENTS

Three syngas qualities (low, medium or high calorific value) can be produced from gasification by varying gasifying agents, method of operation and operating conditions. The main agent is air or air/steam, but oxygen/steam and hydrogen can also be used. Air gasification technology is the simplest and most often used due to the high cost of using other gasification agents and on-site safety issues. In air or steam/air gasification, the fuel gas has low calorific value, usually 4-6 MJ/Nm^3. Using oxygen/steam gives a medium calorific gas of 12-18 MJ/Nm^3 and using hydrogen this gas has high calorific power, around 40 MJ/Nm^3. For low calorific synthesis gas, the purpose is to produce gas engine for heat or electricity generation. Medium or high calorific gas can be used for heat or electricity generation and can also be used for synthesis of liquid fuels (McKendry, 2002c; Castro et al, 2009; Nouh, 2016).

2.2.2.5 RESIDENCE TIME

Residence time influences the quantity and composition of the tars produced. The fraction of oxygen-containing compounds tends to decrease by increasing the residence time. This is a factor that should be analyzed along with temperature. In fixed bed gasifiers the residence time is high, being around 20 minutes. For fluidized bed gasifiers the residence time is less than 1 minute, and depending on the configuration the solid material is recirculated (Lasa et al, 2011; Carvalho, 2012).

2.2.2.6 EQUIVALENCE RATIO

The equivalence ratio (ER) is a key parameter for the gasification process. It is the air/biomass ratio required for gasification divided by the stoichiometric air/biomass ratio required for combustion. The values are less than 1, with an ideal value in the range of 0,2 to 0,3. For ERs lower than 0,2, gasification is incomplete, while for ERs greater than 0,4, gasification is close to combustion. As ER decreases, the concentrations of H_2 and CO in the syngas increase. By increasing the ER, H_2 and CO concentrations decrease while the CO_2 concentration increases, also decreasing the gas heating value. Increasing the ER affects tar breakage due to increased oxygen availability for tar reform reactions (Asadullah, 2013; Lasa et al, 2011; Molino et al, 2018).

2.2.2.7 STEAM TO BIOMASS RATIO

The steam to biomass ratio (SBR) is defined as the ratio between the received steam and the biomass flow feeded. The ideal SBR value for gasification varies up to 1,0. As SBR values increase, H_2, CO_2 and heating value increase, while CO and tar concentrations decrease due to the Water Gas Shift Reaction and to the steam reforming and cracking reactions. However, an excess of steam leads to a reduction in temperature, favoring the formation of tar, and the higher is SBR, the higher is the energy required for the gasification process (Ahmad et al, 2016; Lasa et al, 2011; Molino et al, 2018).

2.3 MODELING OF BIOMASS GASIFICATION PROCESSES

2.3.1 GASIFIER SIMULATION MODELS

In computer simulation, the processes and equipment operate following the sequence of input data, data processing and return output data. Usually this 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 has been spent on incorrect reactor sizing and operation (Li et al, 2001; Abdelouahed et al, 2012).

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. The set of chemical reactions, fluid dynamics, and heat and mass transfer phenomena involved in this process make modeling a complex task. In the case of gasification processes, they can be rigorously modeled by a chemical kinetics approach or approximated by a chemical equilibrium approach. Therefore, gasification models are divided into two main categories: kinetic models and equilibrium models (Li et al, 2001).

2.3.1.1 KINETIC MODELS

Kinetic models employ detailed mechanisms of the chemical reactions present, considering reaction rates, residence time and hydrodynamics. These considerations make this model closer to the reality and are suitable to describe processes at different times and positions in the reactor. However, all these factors increase the complexity of the modeling procedure, due to the number of simultaneous and parallel reactions assumed. The amount of information required may make it difficult to use this type of models, as the accuracy of the data used directly impacts the quality of the predictions obtained (Li et al, 2004; Buragohain et al, 2010).

2.3.1.2 THERMODYNAMIC EQUILIBRIUM MODELS

For equilibrium models, a state of chemical equilibrium is assumed such that the reaction system is in its most stable state (lowest free energy). For this, the main hypothesis considered 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 CO_2 and CH_4, tar and residual carbon fractions are underestimated. There are two types equilibrium models: stoichiometric and non-stoichiometric. The stoichiometric model is based on equilibrium constants, which may limit the study since such constants are restricted to certain temperature and pressure conditions and are not always easily found for all reactions (Rodrigues, 2015).

The non-stoichiometric equilibrium model is based on minimizing Gibbs's 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. It is a simple model and can be used when the molecular formula is not known. Therefore, this non-stoichiometric method is particularly suitable for simulating biomass gasification, as the chemical formula is unknown and the gasification reaction mechanisms are complex (Carvalho, 2012; Rodrigues, 2015; Sun, 2014).

2.3.2 SOFTWARES

In the area of gasification simulation, the main software used in the studies and found in the literature is Aspen Plus (AspenTech). It is the leading chemical process modeling tool in the field of Chemical Engineering being used in modeling, simulation, optimization of industrial chemical processes, sensitivity analysis and economic evaluation. However, there are other gasification modeling and simulation software such as Aspen HYSYS (AspenTech), which is a variation of Aspen Plus, and UniSim Design (Honeywell).

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. This software provides tools very similar to the most commonly used software, but few studies are found in the field of pyrolysis or gasification with UniSim Design.

Some gasification studies and the respective tools are presented in Table 7.

Table 7. Biomass gasification studies.

Biomass	**Gasifier**	**Gasifying agent**	**Software**	**Moisture (%)**	
Pine	CFB	Air and steam	Aspen Plus	8,0	Suwatthikul et al, 2016
Almond shell	CFB	Air and steam	UniSim Design	3,3	Nouh, 2016
Straw	CFB	Air and steam	Aspen Plus	8,5	Shen et al, 2008
Pine	BFB	Air and steam	Aspen Plus	8,0	Nikoo and Mahinpey, 2008
Wood	BFB	Air and steam	Aspen Plus	15,0	Kaushal and Tyagi, 2017
Wood	BFB	Air and steam	Aspen Plus		Beheshti et al, 2015
Rice rusk	Updraft	Air		11,5	Jiang, 2003
Solid waste		Air and steam	Aspen Plus	46,0	Araújo, 2016
Food waste		Air	Aspen Plus	29,3	Razmzan, 2011
Hypothetical	Downdraft	Air	Comsol Multiphysics	0,0	Chaurasia, 2016
Wood	Downdraft	Air	Aspen Plus	16,0	Tavares et al, 2020
Several woods	Downdraft	Air	Aspen Plus	15,0	Keche et al, 2015
Hardwood chips	Downdraft	Air	Aspen Plus	8,9	Han et al, 2017
Palm leaves	Downdraft	Air, steam and O_2	Aspen Hysys	5,0	Bassyouni et al, 2014

For the gasification simulations in a fluidized bed gasifier, air and steam were used as gasifying agents, Aspen Plus and UniSim Design were applied. For bubbling bed gasifiers, the software used was Aspen Plus to simulate wood gasification processes. In downdraft gasifiers, the air was mainly used as a gasifier and again Aspen environment was selected as a computational tool. It is noted that the predominant gasifying agent is air because of the low cost. It is also seen that gasification studies are usually simulated at atmospheric pressure and that the moisture content of the raw material is around 10wt.%. The temperature in all studies ranged from 600 to 1400°C.

2.3.3 GASIFICATION BLOCKS

In the literature, there are studies of modeling and simulation of biomass gasification mainly using Aspen Plus. 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 biomass forest 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.

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 4 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 4 blocks: Biomass, Drying and Decomposition, Combustion, and Gasification (see Figure 8). The Biomass block is where the input of biomass information will be given into the software. In the Drying and Decomposition block, the moisture content is reduced, and the biomass is decomposed into volatile and char compounds. Finally, 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 of the reactions involved in the process.

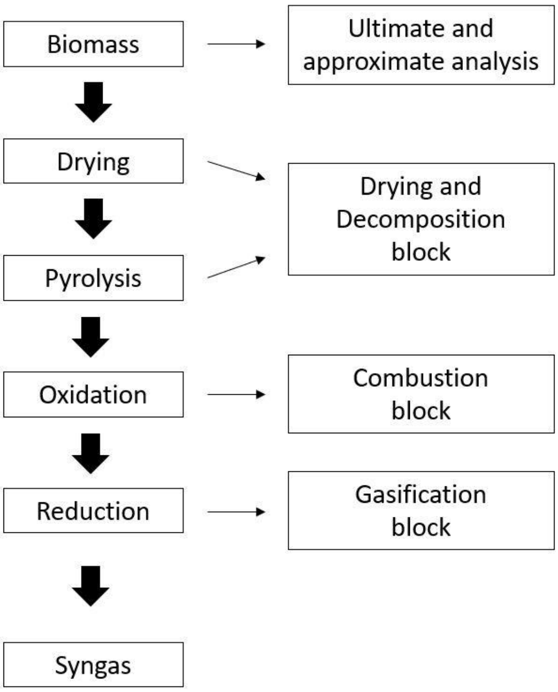


Figure 8. Process flow diagram for modelling gasification processes.

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 coal 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's free energy by calculating the gas composition reaching full chemical equilibrium. In this block, air will be introduced as 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.

Chapter 3 – Model development

3.1 UNISIM DESIGN 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.

3.1.1 ASSUMPTIONS

Some considerations were made for the construction of this model:

1. Process operates in steady state.
2. Operation takes place at atmospheric pressure and all pressure losses are neglected.
3. Char is 100% carbon.
4. Peng-Robinson equation of state was selected as the thermodynamic package for the all process.
5. Air consists of 79% N_2 and 21% O_2 on a molar basis.
6. N_2 is a diluent and an inert, so it does not react.
7. Sulfur (S) and chlorine (Cl) bound to the fuel are converted to hydrosulfuric acid (H_2S) and hydrochloric acid (HCl), respectively.
8. Tar formation is significantly reduced in the process, so it is neglected during the simulation.
9. Biomass feed in the gasifier shows a uniform size distribution.

3.1.2 FEEDSTOCK

The studied selected biomass sources were hardwood chips and almond shells, considered as a hypothetical charcoal simulated from the parameters shown in Table 8. The input values ($kg.h^{-1}$) of air and steam are listed in Table 9, in addition to the conditions of process operation.

Table 8. Approximate and ultimate analysis of the biomass stocks (Schmid et al, 2012; Nouh, 2016).

Biomass Feedstock		**Hardwood chips**	**Almond shell**
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^{-1})		17	18
Flow rate (kg.h^{-1})		5	5

Table 9. Parameters input in simulation study.

Air Feedstock		
Temperature	25	°C
Flow rate	0,3-2,4	kg.h^{-1}
Steam Feedstock		
Temperature	100	°C
Flow rate	0,18-3,6	kg.h^{-1}
Operating condition		
Temperature	600-1200	°C
Pressure	1	atm

3.1.3 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 which constitutes de process. UniSim Design does not consider any form of biomass as a predefined component in its component library. In this way, the biomass was modeled by Python software using the ultimate and approximate analysis to estimate the properties of the decomposed input current.

This inlet stream was calculated considering 100 g of biomass for the calculation basis. To estimate the decomposition, several calculation steps were necessary. First, the mass quantity of each element (C, O, H, N, S, Cl) was determined from the elementary analysis by multiplying the mass fraction of each element by 100. However, for this simulation it was determined that the decomposed material is formed by C, O_2, H_2, N_2, H_2S, HCl, H_2O. Thus, it is necessary to calculate the mass quantity of each of these components. Thus, the mass amount of C and N_2 is equal to the elemental mass amount, however for the components O_2 and H_2 it was necessary to subtract mass amounts that are part of other molecules (H_2S, HCl and H_2O). Therefore, for O_2, the mass amount of O present in H_2O was subtracted from the mass value. For H_2, the mass amount of H present in H_2S, HCl and H_2O was subtracted from the mass value. For the H_2S components, HCl it was necessary to add mass amounts of H according to the number of moles of S and Cl and molar mass of H. And for H_2O, the mass fraction of moisture was multiplied by 100. With all amounts calculated masses, the mass composition of each component was estimated by dividing the mass quantity of each component by the value 100 g of the calculation base.

To estimate the molar composition, it was necessary to first calculate the number of moles of each component by dividing the mass quantity of each component by the molar mass. After that, all moles were added. With all mole numbers calculated and added together, the molar composition of each component was estimated by dividing the molar quantity of each component by the total number of moles. Thus, obtaining the mass and molar composition values of the biomass for complete decomposition, shown in Table 10.

Table 10. Mass and molar composition of decomposed biomass.

	Hardwood chips		**Almond shell**	
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
HCl	0,003	0,001	0,052	0,017
H_2O	5,700	3,823	3,300	2,101

3.1.4 SENSITIVITY ANALYSIS

In this section the model developed for a downdraft gasifier will be studied. The syngas at the end of the process, must be formed by CO, H_2 and variable amounts of CH_4, 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: syngas molar composition, syngas flow and heating value.

3.2 MODEL DESCRIPTION

The process is simulated in 3 main steps: drying and decomposition, combustion and gasification. For this, a Conversion Reactor, Gibbs Reactors, as well as other equipments such as Mixers and Splitters were used. The flowsheet is illustrated in Figure 9.

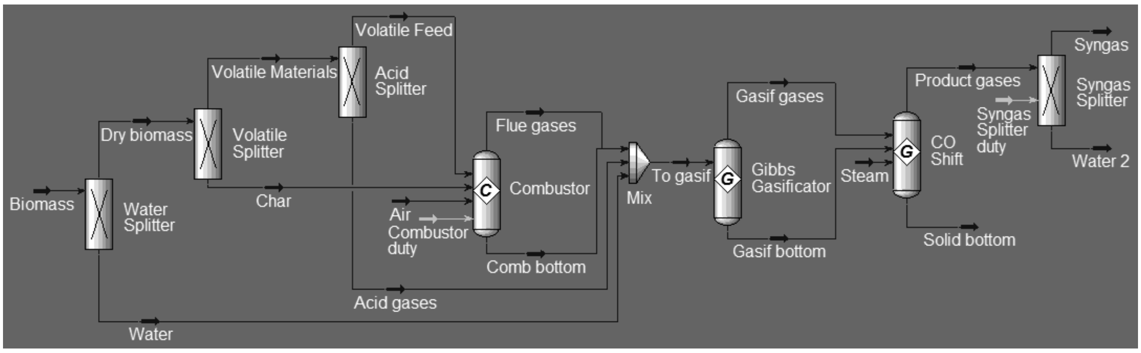


Figure 9. UniSim Design flowsheet for the downdraft gasification process.

3.2.1 DRYING AND DECOMPOSITION

The input current “Biomass” was defined by Python software from the ultimate and approximate analysis, shown in Table 10. This current entered at 500°C in the Splitter equipment, named “Water Splitter” to separate the water present in the current. Thus, having the stream of biomass decomposed into the two streams "Dry biomass" and "Water".

Another Splitter equipment, named “Volatile Splitter” was used to separate volatile materials from coal, 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.

3.2.2 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 the Table 5. For this, a Conversion Reactor equipment was used, named

“Combustor”, which was operated at 1000°C. The input currents in this equipment were “Volatile feed”, “Char” “Air” and “Combustor duty”. From this equipment, the currents "Flue gases" and "Comb bottom" are obtained.

3.2.3 GASIFICATION

Gasification reactions are a set of equilibrium reactions. To facilitate modeling at UniSim Design, the set of reactions was separated into two Gibbs reactors. For feeding in the first reactor, a Mixer equipment, called “Mix”, was used to mix the following currents: “Flue gases”, “Comb bottom”, “Acid gases” and “Water”, thus obtaining a unique current called “To gasif” that enters the first Gibbs reactor. The first reactor was named “Gibbs Gasificator”. The following reactions are simulated in it: Boudouard Reaction (6), Reforming of Char (7), and Hydrogasification (9), according to Table 5. The first two reactions are endothermic and the third one is exothermic. Exiting this reactor are the “Gasif gases” and “Gasif bottom” streams, both of which enter the next reactor, in addition to the “Steam” steam inlet.

The second reactor was named “CO shift”. This is a reactor in which two reactions are modeled: Water Gas Shift Reaction (8) and Steam-methane Reforming (10), according to the Table 5. The first reaction is exothermic and the second one is endothermic. From this reactor, two currents are removed: “Product gases” that enter the next equipment, and the “Solid bottom” current. Finally, there is a “Splitter” device, named “Syngas Splitter” that simulates the removal of water from the gas. This equipment has as input the current "Product gases" and at the output two currents: "Water" and "Syngas". The "Syngas" being the final current, thus obtaining the product gas at the end of the process.

Chapter 4 - Results and Discussion

4.1 REFERENCE CONDITIONS

In this part of the work the model developed for a downdraft gasifier will be studied. The syngas at the end of the process, must be formed by CO, H_2 and small amounts of CH_4, H_2S, HCl and N_2. After discussing the simulated data, a comparison will be made with two case studies selected from the literature.

4.1.1 SIMULATION

For the model developed, a simulation was performed for each of the two biomass sources studied (hardwood chips and almond shell). For this simulation, the steam to biomass ratio was 0,2 for both biomass and the chosen equivalence ratio was 0,4 for hardwood chips and 0,45 for almond shell in which air entered the process at 25°C and steam at 100°C as shown in Table 11.

Table 11. Parameters for the simulation.

	Hardwood chips		**Almond shell**	
	Air	Steam	Air	Steam
ER	0,40	-	0,45	-
SBR	-	0,20	-	0,20
Temperature (°C)	25,0	100,0	25,0	100,0
Molar flow (kmol.h^{-1})	0,042	0,055	0,045	0,055
Mass flow (kg.h^{-1})	1,296	0,991	1,405	0,991

Below are presented the main process currents, temperatures, flows (molar and mass), syngas heating values, and molar compositions, in addition to possible explanations for the variations in the composition of the currents and temperatures in the main stages of the simulation.

Tables 12 and 13 show the main currents of the process, in addition to the main variables studied. The decomposed inlet current "Biomass" enters the process at 500°C with a mass flow of 5 kg.h^{-1} 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” current is the equipment's current output that simulates oxidation reactions. It is seen that the current comes out with a fixed temperature of 1000°C. It is interesting to note that the main reaction favored was Carbon Partial Oxidation (3) due to low air intake, favoring the formation of CO. The other reactions are favored when the amount of air for combustion is greater.

Table 12. Main simulation currents for hardwood chips.

	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^{-1})	0,414	0,329	0,361	0,353	0,412	0,386
Mass flow (kg.h^{-1})	5,000	5,819	6,296	6,296	7,287	6,811
HHV (MJ.kg^{-1})	-	-	-	-	-	14,632
LHV (MJ.kg^{-1})	-	-	-	-	-	13,501
HHV (MJ.m^{-3})	-	-	-	-	-	2,925
LHV (MJ.m^{-3})	-	-	-	-	-	2,699
C	49,618	0,000	4,426	0,000	0,000	0,000
O_2	14,937	0,000	0,000	0,000	0,000	0,000
H_2S	0,006	-	0,007	0,007	0,006	0,006
HCl	0,001	-	0,001	0,001	0,001	0,001
H_2O	3,823	0,000	4,386	0,465	6,408	0,000
CO	-	57,570	52,492	56,488	42,063	44,943
H_2	31,550	39,693	36,192	38,823	41,601	44,449
CO_2	-	0,000	0,000	0,579	7,319	7,819
CH_4	-	-	-	1,085	0,419	0,448
N_2	0,065	2,738	2,496	2,551	2,184	2,334

Table 13. Main simulation currents for almond shell.

	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^{-1})	0,436	0,359	0,383	0,371	0,435	0,410
Mass flow (kg.h^{-1})	5,000	6,059	6,405	6,405	7,396	6,943
HHV (MJ.kg^{-1})	-	-	-	-	-	15,477
LHV (MJ.kg^{-1})	-	-	-	-	-	14,253
HHV (MJ.m^{-3})	-	-	-	-	-	2,923
LHV (MJ.m^{-3})	-	-	-	-	-	2,692
C	48,227	0,000	3,869	0,000	0,000	0,000
O_2	14,239	0,000	0,000	0,000	0,000	0,000
H_2S	0,002	-	0,002	0,003	0,002	0,002
HCl	0,017	-	0,018	0,019	0,016	0,017
H_2O	2,101	0,000	2,389	0,084	5,781	0,000
CO	-	54,392	50,976	54,930	42,028	44,606
H_2	35,328	42,868	40,176	40,536	43,625	46,301
CO_2	-	0,000	0,000	0,080	5,921	6,284
CH_4	-	-	-	1,693	0,365	0,387
N_2	0,086	2,741	2,569	2,656	2,263	2,402

The next stream is “To gasif” where all the previous currents come together. This is the current that enters the first reactor that simulates the reduction reactions. The temperature decreases a little in relation to the current that leaves the combustion due to the lower temperatures of the other currents, entering in thermal equilibrium. In this current there is the char that has not been volatized, the acid gases, in addition to the current that comes from the combustor. Therefore, a high amount of C is noted due to the char, the presence of water due to the biomass moisture and also the gases already formed from CO, H_2 and inert N_2.

The “Gasif gases” current is the output current of the first equipment that simulates the reduction reactions. In this current it is noted that there was an increase in the composition of CO, in addition to the formation of CH_4 and all consumption of C. This is due to a favoring of reactions Reforming of Char (7) and Hydrogasification (9). The reaction (9) is exothermic and the reaction (7) endothermic, however the Reforming of Char reaction has an enthalpy 2,3 times higher, thus the temperature in this area of the gasifier reduces in relation to the current that entered because there was a higher consumption of energy compared to the energy released by the exothermic reaction.

The “Product gases” current is the output current of the second reactor that simulates the reduction reactions. It is seen that the temperature has declined in relation to the input current. Also, it is 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 gasifier 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 5 times greater. 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” output current has high compositions of CO and H_2, close to 45% and low compositions of the other components (H_2S, HCl, CH_4 and N_2). Only CO_2 showed a formation between 6 to 7%. However, with the steam input, it is inevitable a favoring of the Water Gas Shift Reaction (8) and consequently the formation of CO_2. The entry of steam promotes the formation of H_2, but it also has the problem of favoring the formation of CO_2. Therefore, one must work with a low steam value in order to avoid this difficulty.

4.1.2 LITERATURE

In this section, the results of two studies of biomass gasification in the literature (Nouh, 2016; Han et al, 2017) will be presented and discussed (see Table 14) and later compared to the study done above. One of the studies is the gasification of hardwood chips and the other of almond shell. The first work (Nouh, 2016) was the simulation of the gasification of almond shell, however the simulated gasifier was a fluidized bed gasifier. The gasifying agent used was air and steam. The study was carried out using the chemical process software UniSim Design. The pressure varied between 1 to 3 atm and the temperature varied between 700 to 1100°C. In the analysis of air intake, a decrease in CO and H_2 was observed with a rise in air flow. Another parameter analyzed was steam, with the increase in steam reduce the CO composition and raise the H_2 composition. The behavior of syngas in relation to temperature was of growth the composition of CO and H_2.

The second work (Han et al, 2017) is a simulation of the gasification of hardwood chips in a downdraft gasifier. 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 behavior of the syngas compositions was a decrease in CO, H_2 and CH_4 with a raise in ER, and an increase in CO_2 with a raise in ER. The behavior of the syngas composition in relation to the rise in the gasifier temperature was an increase in CO and a reduction in CO_2 and CH_4. H_2 behaved in such a way that even the temperature of 750°C had its value increased and after that the H_2 composition declined. It is concluded that the recommended temperature for gasification is between 650 to 800°C and the equivalence ratio 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 removal and N_2 of the composition of hardwood chips is made, the amount of CO would be 41,54 %, H_2 35,58 %, CH_4 0,39 % and CO_2 22,48 %. As excess air was used to obtain this syngas current, considerable 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 output composition of the synthesis gas produced.

Table 14 shows that the outlet gas compositions diverged from the almond shell study, where the amount of CO was higher (approximately 30%) compared to our study and H_2 was lower (approximately 50%). It may be due to the fact that you have worked with a low amount of steam. The study of hardwood chips was closer in terms of composition. When removing N_2 from the composition, note that CO differs 8% and H_2 20%. It is also seen that there is a large amount of CO_2 (22,48%), compared to our study (7,82%). As previously discussed, this high presence of CO_2 is due to the fact that a large amount of air is used to carry out the process.

Table 14. Parameters and results of reference studies (Han et al, 2017; Nouh, 2016).

Studies	**(Han et al, 2017) model**	**Our model**	**(Nouh, 2016) model**	**Our model**
Type of biomass	Hardwood chips	Hardwood chips	Almond shell	Almond shell
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
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
CH_4 (%)	0,20 (0,39)	0,45	6,12	0,39
N_2 (%)	48,99 (0,00)	2,33	8,29	2,40

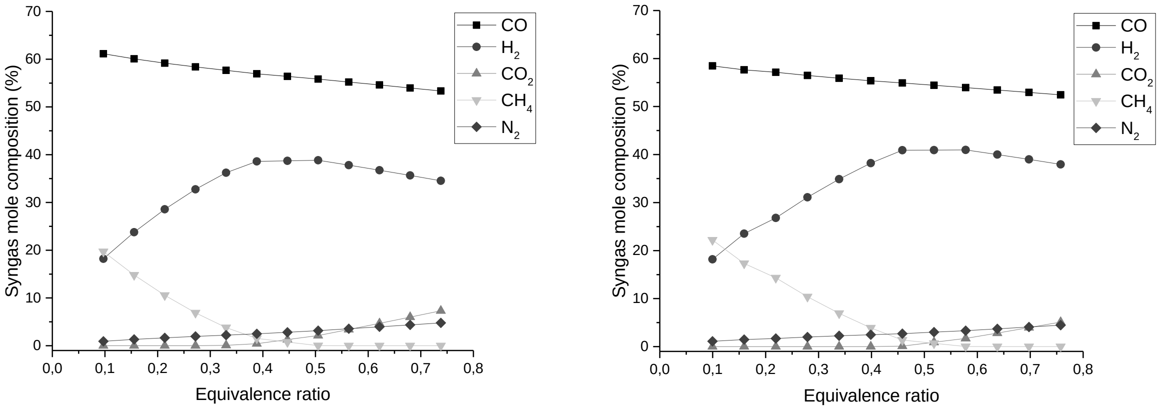
Note that both ER and SBR are parameters that significantly change the composition of the outlet gas. For the simulations that will be presented below, low air intakes were applied in order to avoid CO_2 formation, in addition to analyzing whether the steam input significantly interferes with the expected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

4.2 EFFECT OF EQUIVALENCE RATIO

In this stage, the study of the influence of the air intake on the syngas composition, heating value and gasification temperature is presented. Here the ER is the independent variable, with the syngas molar composition, syngas flow, heating value and gasification temperature as dependent variables. For this study, the biomass input is fixed at 5 $kg.h^{-1}$. In addition, the air intake was varied up to 2,4 $kg.h^{-1}$ (approximately 0,8 ER) and there was no steam entry in the process, only the water present in the biomass moisture was used.

4.2.1 SYNGAS MOLE COMPOSITION

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 increases, the amount of oxygen supplied to the gasifier also increases, providing a greater conversion of the carbon present in the fuel. However, an excessive amount of oxygen completely oxidizes the fuel and the production of syngas declines. Therefore, ER is an essential parameter in the gasification process. (Ramzan et al, 2011; Lasa et al, 2011; Ahmad et al, 2016; Han et al, 2017). Figure 10 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 which are 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 N_2 that rise with increasing air intake. However, in the ER close to 0,4, for hardwood chips and 0,5, for almond shell, 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 H_2 values, high CO composition and virtually zero CO_2 composition. For ER values below 0,2, gasification is incomplete, and above 0,5, gasification is similar to combustion, with the increasing formation of CO_2.



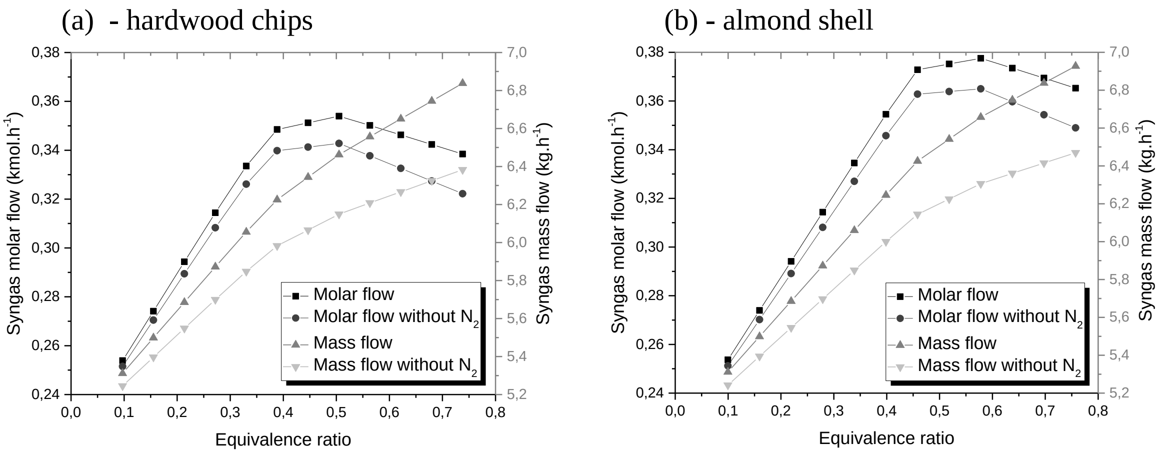
(a) - hardwood chips

(b) - almond shell

Figure 10. Effects of ER on syngas composition for hardwood chips (a) and almond shell (b).

4.2.2 SYNGAS MOLAR AND MASS FLOW

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 the molar and mass quantities of this production were studied. In this section, the behavior of syngas production was analyzed due to the increase in the equivalence ratio. As the independent variable is the air intake, the behavior of the flows was also analyzed, removing N_2 from the final current. Therefore, Figure 11 shows the behavior of the molar and mass flow as a function of the equivalence ratio for both studied biomasses. It is seen that the mass flow rises with increasing air intake. This is expected because a greater amount of air promotes the formation of H_2 and after 0,4 ER the formation of CO_2, in addition to increasing the amount of inert gas N_2. When the N_2 is removed from the mass flow, there is a diminishing of approximately 1% in low ER and approximately 6% in high ER. The molar flow increases up to approximately 0,4 ER for hardwood chips and 0,5 for almond shell, 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 H_2 and a rise in CO_2. As the molar mass of CO_2 is greater than the molar mass of H_2 (44,010 $g.mol^{-1}$ and 2,016 $g.mol^{-1}$, respectively), a greater mass of CO_2 gas is required to obtain the same molar amount of H_2. This behavior is seen in the curves at the moment when H_2 starts to decrease 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 decrease in the production of molar syngas by approximately 1% in low ER and 4% in high ER.

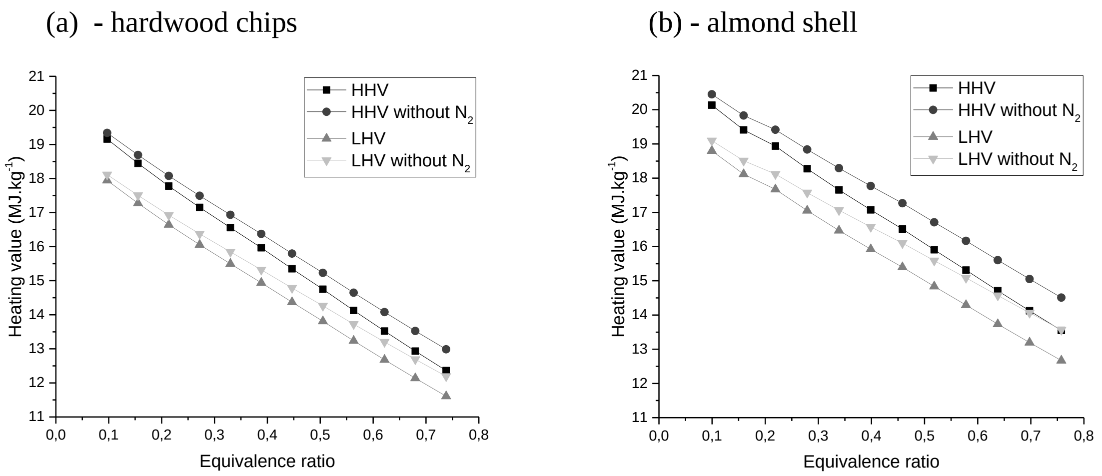

(a) - hardwood chips

(b) - almond shell

Figure 11. Effects of the ER on syngas molar and mass flow for hardwood chips (a) and almond shell (b).

4.2.3 HEATING VALUE

The heating value of a product gas is a measure of quality. This heating value decreases as more air is supplied (Mansaray et al, 1999; Li et al, 2001). Figure 11 shows the behavior of the high and low heating values due to the increase 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 rise in air in the process causes it to have a greater amount of N_2 in the synthesis gas, in addition to favoring the formation of CO_2. If N_2 is removed from the synthesis gas, there is an increase 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 increase in CO_2 is the factor that most affects the calorific value. Thus, the heating value of the gas diminish with the rise in the ER.


(a) - hardwood chips

(b) - almond shell

Figure 12. Effects of ER on heating value for hardwood chips (a) and almond shell (b).

4.2.4 GASIFIER TEMPERATURE

Usually the gasification temperature is analyzed as an independent variable depending on the composition of the synthesis gas (Silva et al, 2014; Bassyouni, 2014). However, it is interesting to analyze the temperature behavior of the gasifier when considering the temperature as a dependent variable. Figure 12 shows how the temperature in the reactors behave with the increase 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 shell, the gasification temperature decline with increasing 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 present heat causing the temperature to decrease. From that value (0,4 and 0,45), the temperature starts to rise. 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.

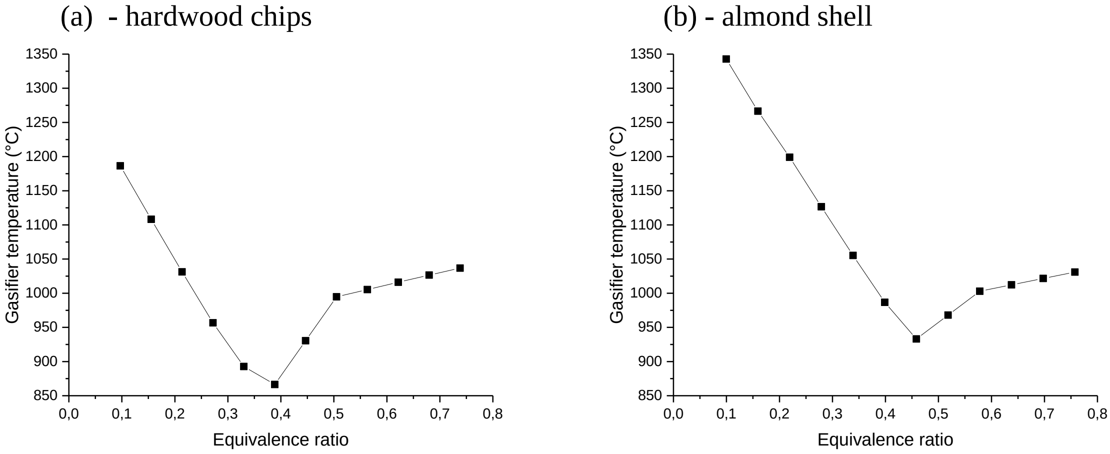


Figure 13. Effects of ER on gasifier temperature for hardwood chips (a) and almond shell (b).

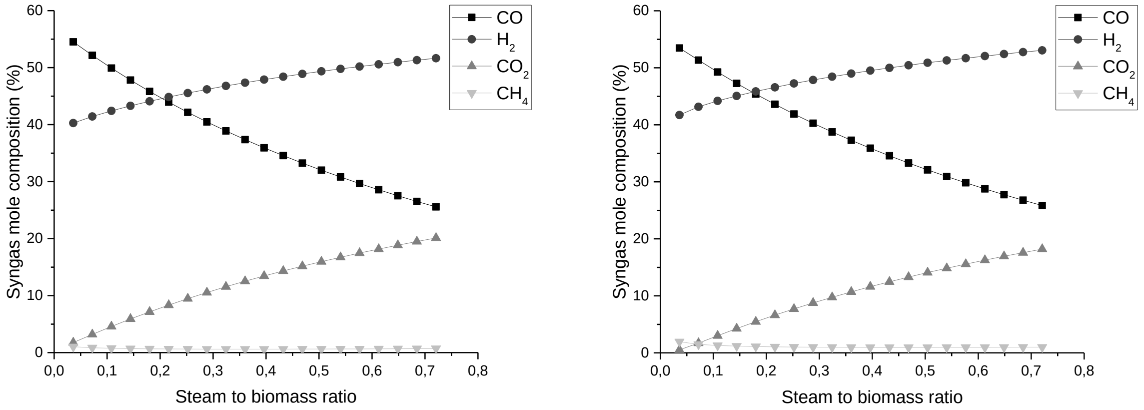
4.3 EFFECT OF STEAM TO BIOMASS RATIO

In this section, the study of the influence of steam input on the syngas composition, heating value and gasification temperature will be made. Here the SBR is the independent variable, with the syngas molar composition, syngas flow, heating value and gasification temperature as dependent variables. For this study, the biomass input is fixed at 5 kg.h^{-1}. In addition, the steam intake was varied up to 3,6 kg.h^{-1} (approximately 0,7 SBR) and the air intake was fixed at 1,25 kg.h^{-1} (approximately 0,4 ER).

4.3.1 SYNGAS MOLE COMPOSITION

The steam to biomass ratio is the ratio of the steam flow to the biomass flow. This is an important parameter in the gasification process as it is directly linked to the formation of H_2. The increase in steam in the reactor favors H_2 formation reactions, especially Water Gas Shift Reaction (8) and Steam-methane Reforming (10). However, it also ends up favoring the formation of CO_2. Thus, it is necessary to define the best reason for not having unwanted amounts of CO_2 in the synthesis gas (Shen et al, 2008; Bach et al, 2019; Ugwuodo et al, 2020). Figure 13 shows the behavior of the syngas composition as the steam to biomass ratio rises. Both biomasses showed similar behavior. The increase in steam causes the amount of carbon monoxide and methane to diminish. 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.



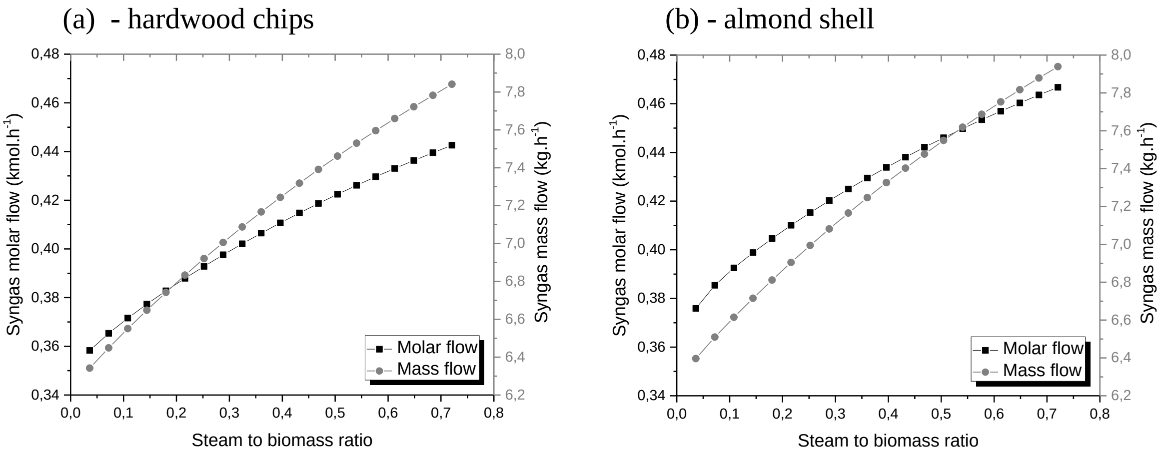
(a) - hardwood chips

(b) - almond shell

Figure 14. Effects of SBR on syngas composition for hardwood chips (a) and almond shell (b).

4.3.2 SYNGAS MOLAR AND MASS FLOW

It is also important to analyze the production of syngas in relation to the entry of steam into the gasifier. Thus, the influence of steam on the molar and mass amount of syngas flow was studied. Figure 15 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 production and molar syngas increase with increasing SBR. This can be explained by the fact that the increase in steam promotes the formation of H_2 and CO_2 mainly because of the Water Gas Shift Reaction (8). And this causes the mass production to rise with the increase in SBR. Regarding molar production, the increasing behavior can be explained by the fact that regardless of the SBR value analyzed, the amount of H_2 and CO_2 is always increasing, with no change in the behavior of the molar composition of syngas (CO and H_2), that are always growing, without growth and then declining in H_2 (seen in the ER study), making the production of syngas also perform in a similar way.



(a) - hardwood chips

(b) - almond shell

Figure 15. Effects of SBR on syngas molar and mass flow for hardwood chips (a) and almond shell (b).

4.3.3 HEATING VALUE

The heating value of the synthesis gas decreases with the increase of steam in the gasification process (Sun, 2014; Bach et al, 2019). As can be seen in Figure 14, the behavior for both biomasses was similar to 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 greater amount of steam provides a greater 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 less. 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, this causes the calorific value to decay. Therefore, a diminishing in CO and an increase in CO_2 causes the calorific value, both higher and lower, to be lower.

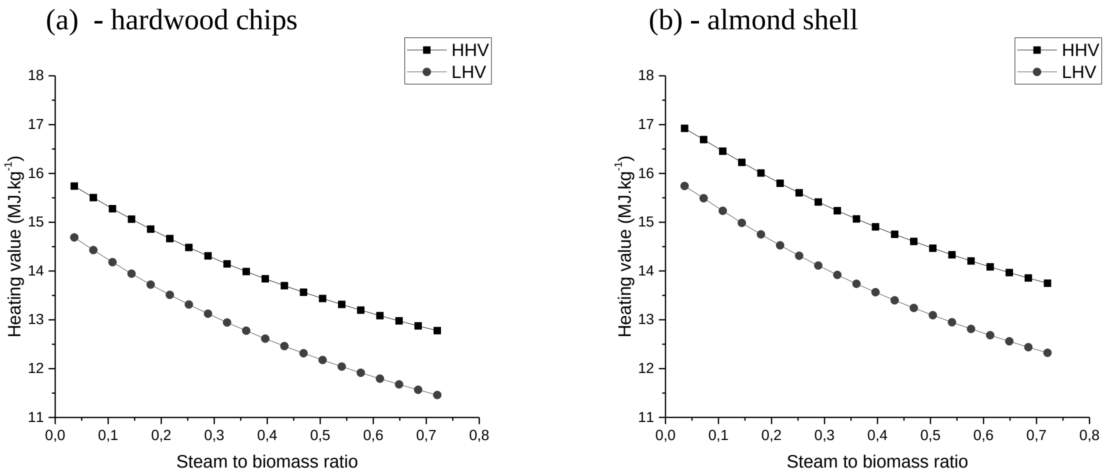


Figure 16. Effects of SBR on heating value for hardwood chips (a) and almond shell (b).

4.3.4 GASIFIER TEMPERATURE

Again, analyzing the behavior of temperature as a dependent variable due to the increase in the amount of steam in the reactors. The expected behavior for increasing the steam to biomass ratio is to decrease the gasification temperature (He et al, 2012). As you can see in Figure 15, the rise in steam input in the reactors decreases the gasification temperature in 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 5 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 seen is that of reducing the temperature with the increase of steam entering the reactor.

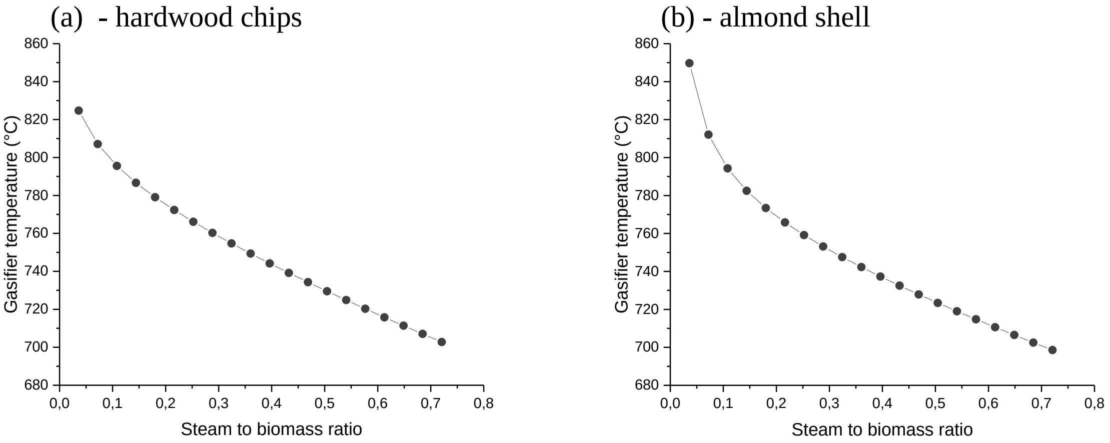


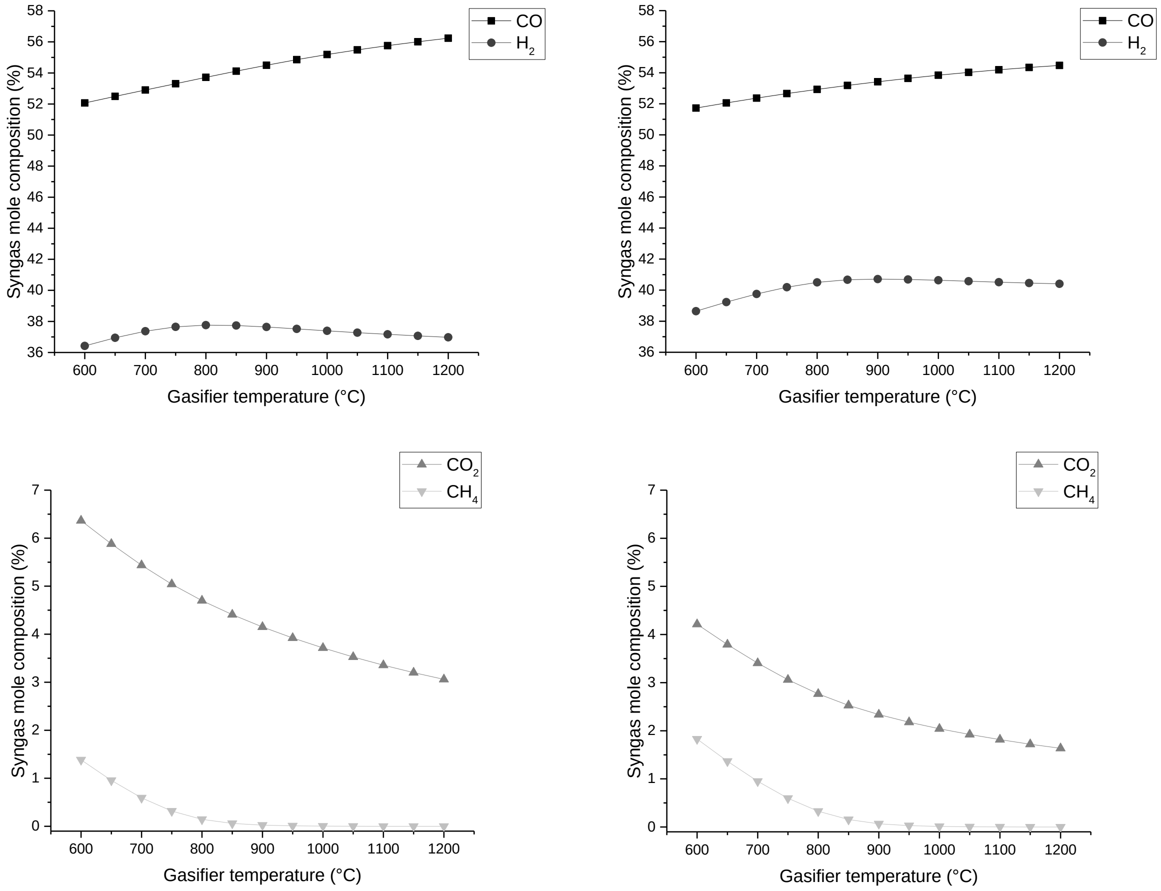
Figure 17. Effects of SBR on gasifier temperature for hardwood chips (a) and almond shell (b).

4.4 EFFECT OF GASIFIER TEMPERATURE

In this step, the analysis of the influence of the gasification temperature on the molar composition and the heating value of the syngas will be carried out. Here, the gasification temperature is the independent variable, with the syngas composition, syngas flow and heating value as dependent variables. For this study, a biomass input of 5 kg.h^{-1} is fixed. In addition, the gasification temperature was varied from 600 to 1200°C, the air intake was fixed at 1,25 kg.h^{-1} (approximately 0,4 ER) and there was no vapor entry, only the water present in the biomass moisture was used.

4.4.1 SYNGAS MOLE COMPOSITION

The gasification temperature is another important parameter in the syngas production process. Hydrogen is expected to increase with the temperature reaching the maximum and then gradually decrease at higher temperatures. Gasification is generally satisfactory at a temperature of 800°C (Lasa et al, 2011; Sun, 2014; Han et al, 2017). Figure 16 shows the behavior of the molar composition of the synthesis gas with the increase in the gasifier temperature for both biomasses. CO has a rise, H_2 increases to the maximum and then decline with increasing temperature. CO_2 and CH_4 decreases. 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. Thus, more CO_2 and CH_4 will be consumed and more CO will be produced. The reactions of Water Gas Shift Reaction (8) and Hydrogasification (9) are exothermic, so a higher temperature makes the reaction more difficult and produces less CO_2, H_2 and CH_4. 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 form CO_2 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°C the reactions may be limited due to the lack of reagents such as CH_4 and H_2O. Thus, the combined effects of the reactions 7, 8, 9 and 10 can cause a diminishing in hydrogen after 800°C.



(a) - hardwood chips

(b) - almond shell

Figure 18. Effects of gasifier temperature on syngas composition for hardwood chips (a) and almond shell (b).

4.4.2 SYNGAS MOLAR AND MASS FLOW

The production of syngas was also analyzed as a dependent variable using the gasifier temperature as the independent one. Thus, the influence of temperature on the molar and mass production of syngas was studied. Figure 19 shows the behavior of the molar and mass flow of the syngas as a function of the gasifier temperature for both biomasses. It is noted that the influence of temperature is small in the production of syngas. In the molar flow the influence is approximately 1% for hardwood and chips and 3% for almond shell. The mass flow influence is approximately 2% for hardwood chips and 1% for almond shell. Mass production decreases depending on the gasifier temperature. This reduce can be explained by the fact that at higher temperatures, there is a slight disadvantage of the Water Gas Shift Reaction (8), causing a minimum balance shift to favor the production of CO and H_2O. As H_2O is separated from the final syngas stream, there is a minimal decline in the syngas mass flow. The molar production of syngas also decreases with increasing temperature in the gasifier. This can be explained by the fact that at higher temperatures there is a slight fluctuation in the H_2 composition caused by the combination of the reactions 7, 8, 9 and 10 causing the H_2 to decrease and because the H_2 molar mass is small, a negative fluctuation of the H_2 composition causes a diminishing in the molar flow of the syngas.

(a) - hardwood chips

(b) - almond shell

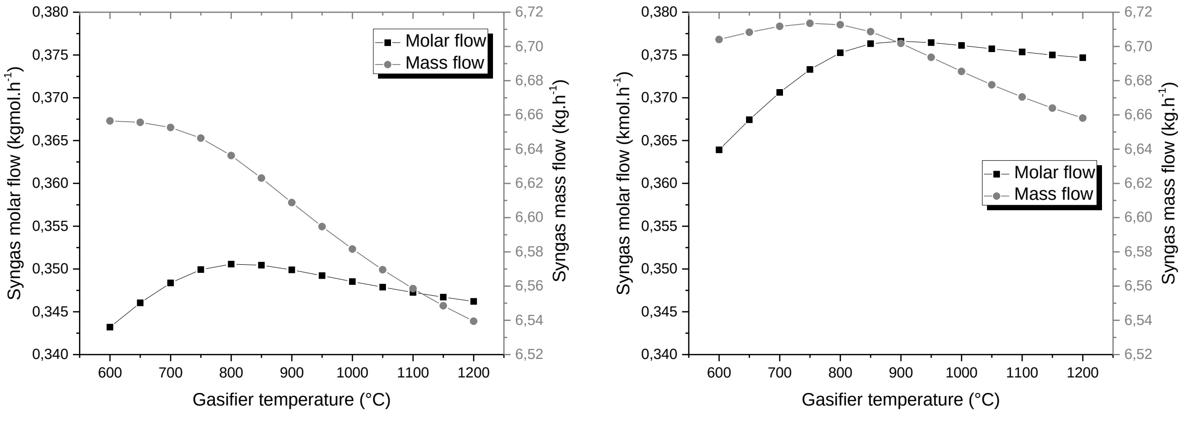
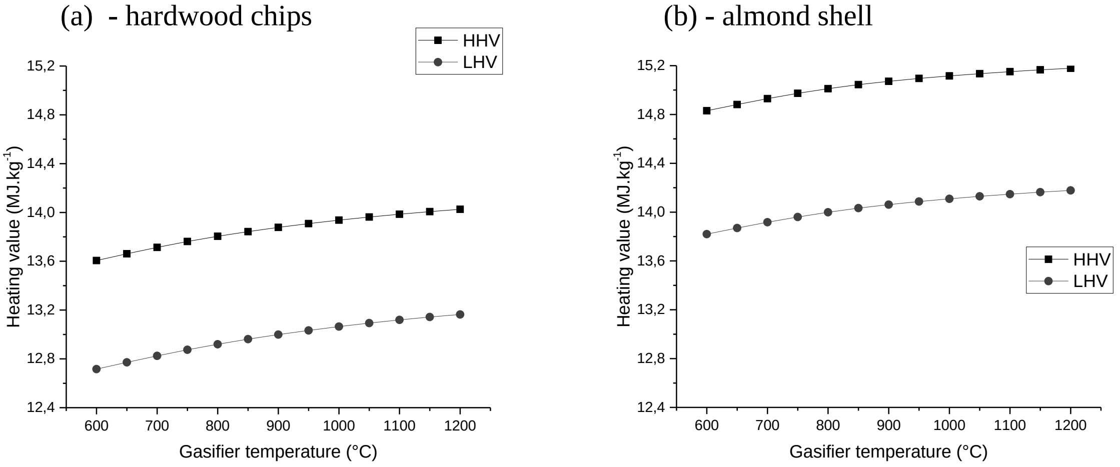


Figure 19. Effects of gasifier temperature on syngas molar and mass flow for hardwood chips (a) and almond shell (b).

4.4.3 HEATING VALUE

The heating value tends to surge with increasing temperature in the gasifier since a growth in the composition of H_2 and CO in the synthesis gas is expected (Li et al, 2004; Bach et al, 2019). Figure 17 shows the behavior of the heating value when the temperature is varied for both biomasses. It is noticeable the increase in the heating value with the rise in the gasification temperature (approximately 4% for hardwood and 3% for almond shell). This is due to the fact that an increase in temperature favors the formation of H_2 and CO in the syngas, rising the calorific value. Even with the stabilization and minimum decline of hydrogen after the temperature 800°C, the CO continues to increase and a greater amount of CO in the syngas causes the energy release by the syngas to be higher, thus the growth of CO tends to increase the heating value.


(a) - hardwood chips

(b) - almond shell

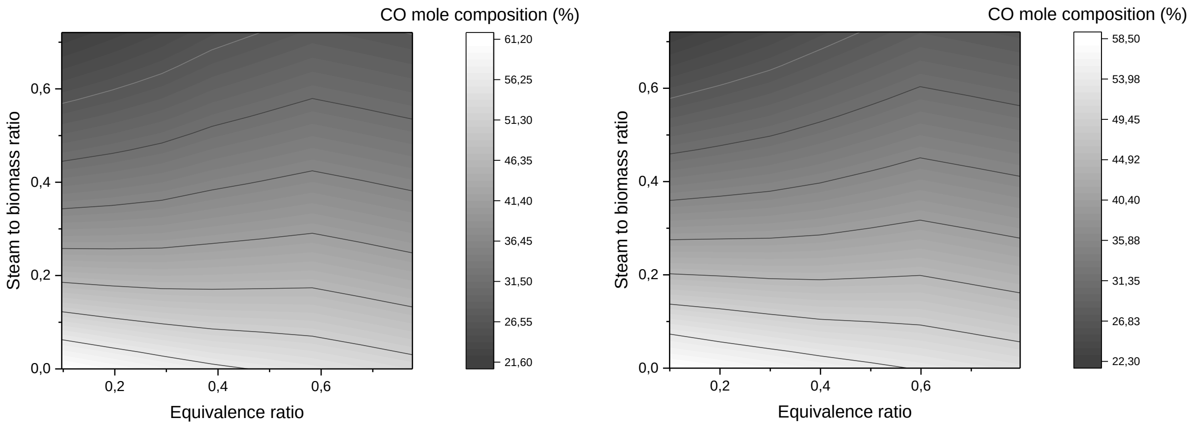
Figure 20. Effects of gasifier temperature on heating value for hardwood chips (a) and almond shell (b)

4.5 COMBINATION EFFECT OF EQUIVALENCE RATIO AND STEAM TO BIOMASS RATIO

The intention of this step is to use the independent variables Equivalence ratio and Steam to biomass ratio to analyze the behavior of the syngas composition, syngas flow and the gasification temperature. Thus, the air intake was varied up to 2,4 $kg.h^{-1}$ (approximately 0,8 ER), steam up to 3,6 $kg.h^{-1}$ (approximately 0,7 SBR) and the biomass intake remained fixed at 5 $kg.h^{-1}$. Thus, it is expected to find maximum and minimum parameters of these independent variables in order to obtain a synthesis gas rich in CO and H_2.

4.5.1 CARBON MONOXIDE

The analysis of ER and SBR previously showed that both the rise in air and the increase in vapor decrease the composition of CO in syngas. Figure 18 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 increase in ER and SBR reduce the composition of CO due to favoring the formation of H_2 and CO_2. It is necessary to analyze the other compositions to find the best combination of ER and SBR, however it is seen that these values must be up to 0,5 (ER) and 0,2 (SBR), because combinations with values greater than these considerably decrease the CO composition in syngas.



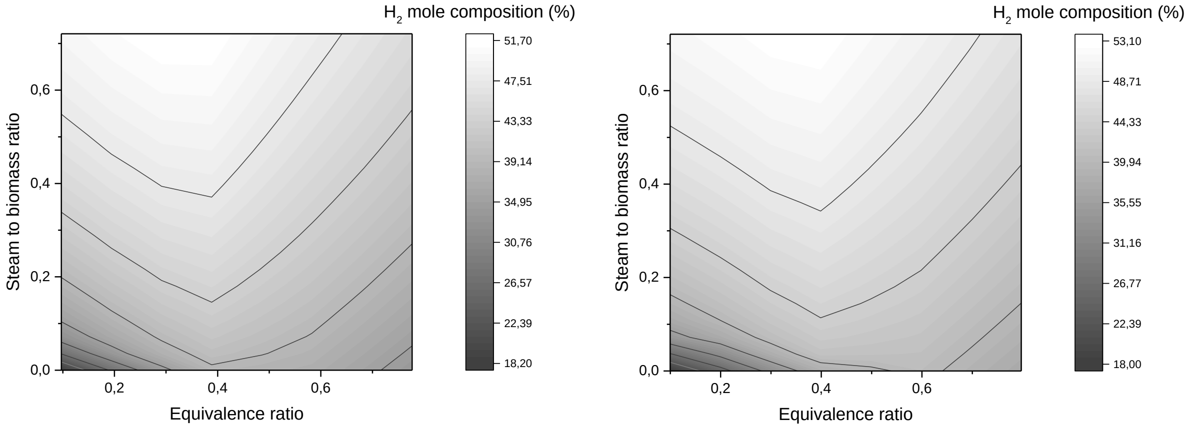
(a) - hardwood chips

(b) - almond shell

Figure 21. Combination effects of ER and SBR on CO composition for hardwood chips (a) and almond shell (b).

4.5.2 HYDROGEN

The ER study previously showed that the rise in air first increases the amount of H_2 and after 0,4 and 0,5 (for hardwood chips and almond shell, respectively) that amount decreases. The SBR analysis showed that the surge in steam increases the composition of H_2 in the syngas. Figure 19 shows how the combination of these two parameters affects the composition of H_2 for both biomasses. It is seen that the rise of ER up to 0,4 in the first graph and 0,5 in the second graph causes the H_2 to growth and after that value there is a decay of the composition. The increase in steam favors the formation of H_2, obtaining compositions greater than 50%. It is observed that for both graphs the best values for obtaining a syngas rich in H_2 is an ER between 0,3 and 0,5 because the lack of air or the excess causes the H_2 to decrease. The entry of steam favors the formation of H_2, but it also favors the formation of CO_2 and reduces the composition of CO. Therefore, it is necessary to analyze the CO_2 composition to choose the best SBR input parameter.



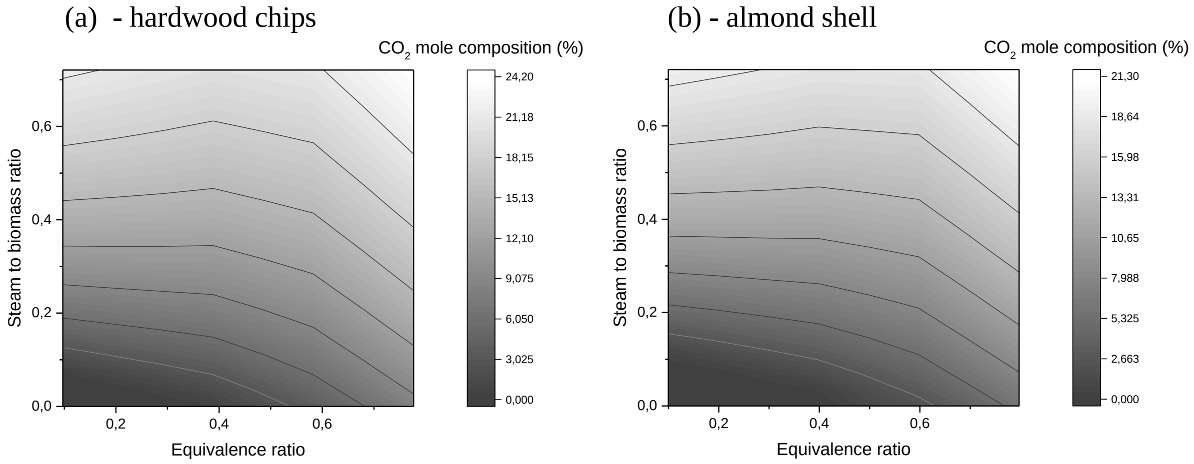
(a) - hardwood chips

(b) - almond shell

Figure 22. Combination effects of ER and SBR on H_2 composition for hardwood chips (a) and almond shell (b).

4.5.3 CARBON DIOXIDE

From the ER and SBR analyzes previously studied, it can be seen that both the rise in air and the increase in steam favor the formation of CO_2. Figure 20 shows the behavior of the CO_2 composition in the synthesis gas when these two parameters are combined for the two studied biomasses. It is seen that the higher the ER and SBR, the greater the amount of CO_2 in the syngas. Therefore, the best range for working with air and steam is up to 0,5 (ER) and 0,2 (SBR).



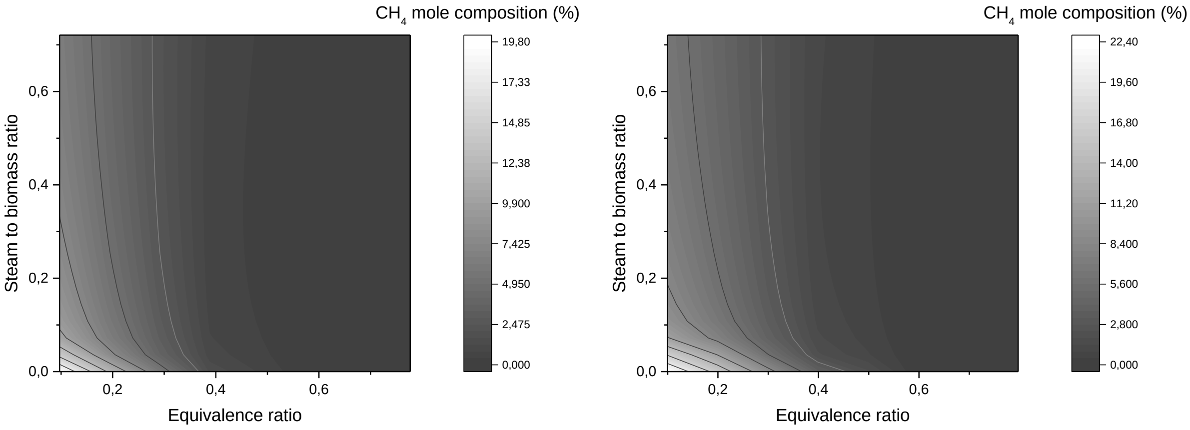
(a) - hardwood chips

(b) - almond shell

Figure 23. Combination effects of ER and SBR on CO_2 composition for hardwood chips (a) and almond shell (b).

4.5.4 METHANE

The ER and SBR studies showed that the increase in air and steam diminish the amount of CH_4 in the synthesis gas. Figure 21 shows the combination of these two parameters in the influence of CH_4 composition for both biomasses. It can be seen that an equivalence ratio of 0,4 is already sufficient to reduce CH_4 in syngas to almost zero. It is also seen that the increase in steam influences the decrease in CH_4. A combination of 0,3 to 0,5 of ER with 0,2 of SBR is sufficient for the practically total consumption of CH_4, thus favoring the formation of CO and H_2.


(a) - hardwood chips

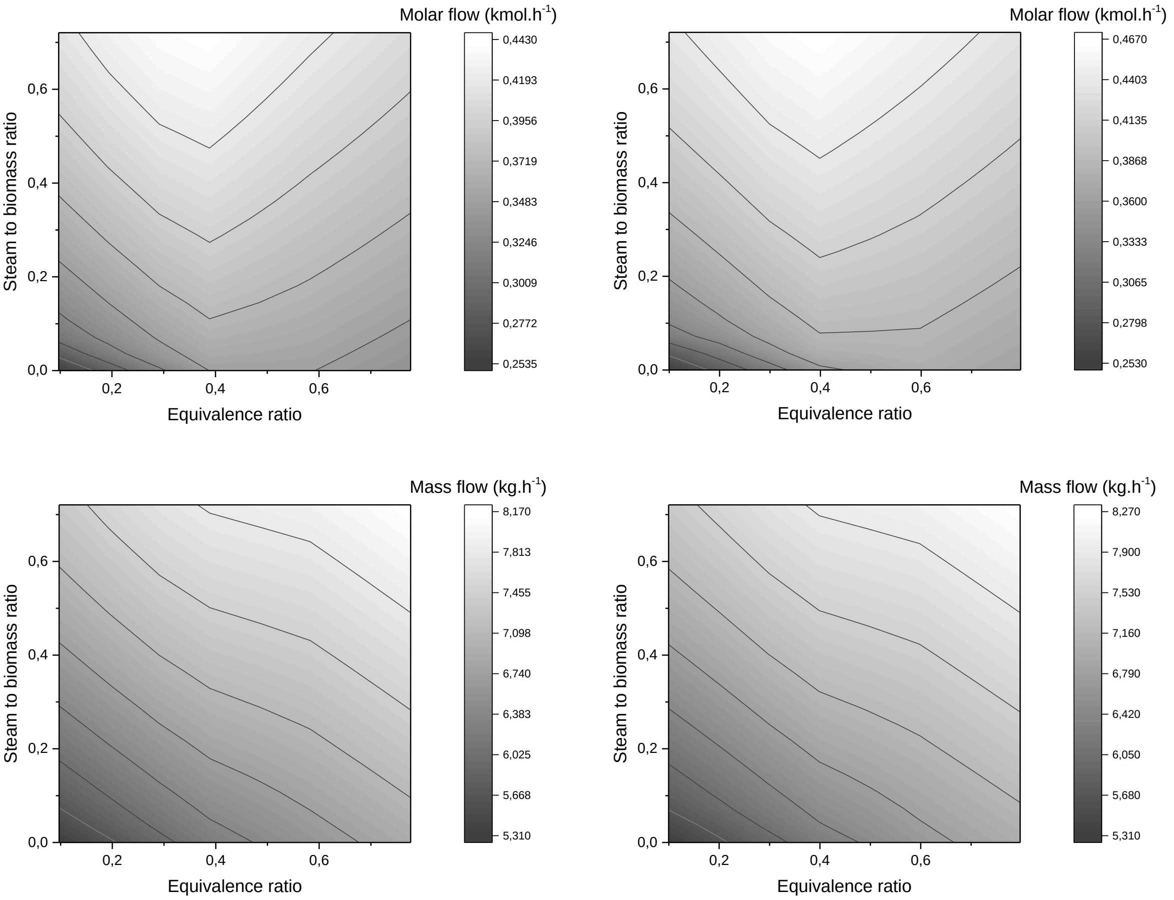
(b) - almond shell

Figure 24. Combination effects of ER and SBR on CH_4 composition for hardwood chips (a) and almond shell (b).

4.5.5 SYNGAS MOLAR AND MASS FLOW

The ER study previously showed that the rise in air first growth the molar flow of syngas and after 0,4 and 0,5 (for hardwood chips and almond shell, respectively) this flow decreases. Regarding the mass flow, there is a surge in value, regardless of the ER. The SBR analysis showed that the increase in steam rises the molar and mass flow. Figure 25 shows how the combination of these two parameters interferes in the molar and mass production of syngas for both biomasses. It is seen that the increase of ER up to 0,4 for hardwood chips and 0,5 for almond shell, in the molar flow graphs, causes the flow to rise and after that value there is a decay of the molar flow. The increase in steam favors the molar production of syngas. Note that for both molar graphs, the best values for greater molar flow are between 0,3 and 0,5 due to the fact that the lack of air or the excess causes H_2 to decline and consequently the molar flow as well. The entrance of steam favors the molar production of syngas. However, the increase in SBR in addition to rising the composition of H_2, increases the composition of CO_2.

It is also observed that the mass flow graphs show that the increase of both ER and SBR increases the mass flow of syngas. As seen in the molar graphics, after 0,4 and 0,5 (hardwood chips and almond shell) of ER there is a reduce in molar flow caused by the decrease in H_2 and the rise in SBR increases the composition of H_2 but also increases the composition of CO_2. Thus, although the ER and SBR rise the syngas mass flow, this flow may not have the best compositions of H_2 and CO. Therefore, in relation to the production of syngas, it is recommended to work with the ER between 0,3 and 0,5 and low SBR.

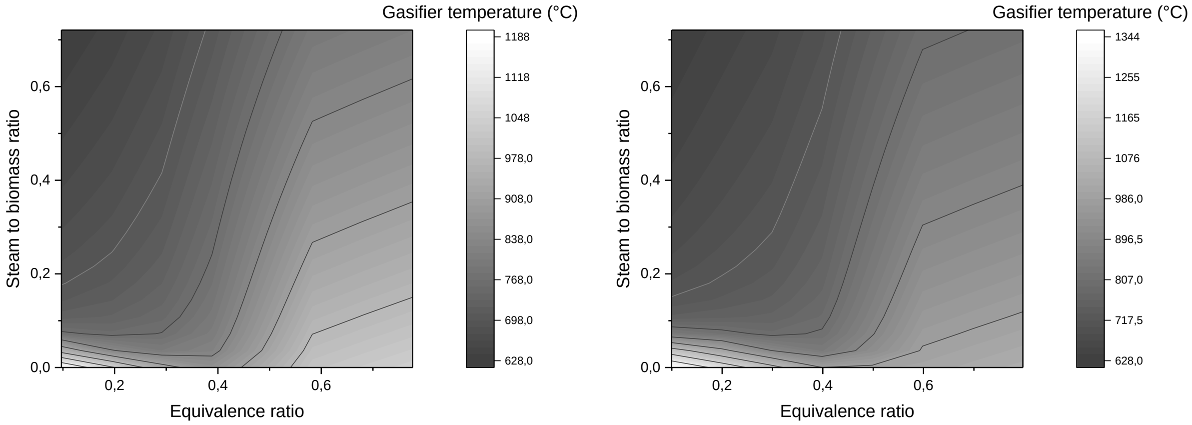

(a) - hardwood chips

(b) - almond shell

Figure 25. Combination effects of ER and SBR on syngas molar and mass flow for hardwood chips (a) and almond shell (b).

4.5.6 GASIFIER TEMPERATURE

The SBR analysis showed that the increase in steam decreases the gasification temperature. The ER study previously showed that the increase in air initially lowers the gasification temperature and after 0,4 for hardwood chips and 0,45 for almond shell the temperature starts to rise. Figure 22 shows the combination of these two parameters in the influence of the reaction temperature for both biomasses. The behavior of increasing steam in decreasing temperature was evident in 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 seen that from the steam to biomass ratio of 0,1 to the gasification temperature since the beginning of the air intake, the temperature does not decline to ER of 0,4 and 0,5 (for hardwood and almond shell, respectively). This can be explained by the fact that the steam input ends up favoring the formation reactions of H_2 Water Gas Shift Reaction (8) and Steam-methane Reforming (10) more than the others. And as Steam-methane Reforming is endothermic with an enthalpy 5 times greater than the Water Gas Shift Reaction, the tendency is for the gasification temperature to decrease.


(a) - hardwood chips

(b) - almond shell

Figure 26. Combination effects of ER and SBR on gasifier temperature for hardwood chips (a) and almond shell (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 to 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 to 950°C.

Chapter 5 – Conclusion and Future Works

5.1 CONCLUSIONS

In this work, a downdraft gasifier was modeled and simulated for two residual biomasses (forest and agricultural) in order to predict the syngas composition. The reactors simulated gasification by minimizing Gibbs free energy. 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 syngas composition, syngas flow and heating value 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:

- Increasing the gasification temperature rises the amount of H_2 and CO while CO_2 and CH_4 diminish.
- The favorable temperature of the gasifier must be between 850 and 950°C, controlling the entry of air and steam to obtain these values.
- The mass flow of syngas rises with the increase in ER and SBR.
- The molar flow surges with the increases of the SBR, however it has an increasing and later decreasing behavior with the rise of ER.
- The heating value of syngas declines with increasing ER and SBR, but increases with rising gasification temperature.
- The contents of H_2 and CO_2 growth with the increase in the steam to biomass ratio, while CO decreases continuously.
- The value of up to 0,2 SBR is an acceptable value to rise the production of H_2 without there being so much CO_2 formation in the syngas.
- The equivalence ratio is a key parameter in the process as it favors the production of H_2. A low amount causes no gasification and a high amount causes CO_2 formation, CO decrease and the presence of N_2 in the synthesis gas.
- An ER of 0,3 to 0,5 is within the favorable range to maximize the amount of CO and H_2 in the process.

In summary, with a temperature between 850 and 950°C, SBR up to 0,2 and ER between 0,3 to 0,5, the best operating conditions are obtained for maximize the composition of the syngas rich in CO and H_2.

5.2 FUTURE WORKS

To complete and continue the work, a few selected tasks are suggested:

- Evaluate the treatment needs of syngas produced for energy applications.
- Evaluate the performance of the model for other sources of biomass.
- Develop an economic study of the energy production of syngas analyzing the profitability of gasification in the face of fixed expenses.
- Develop an economic study of the gasifier production on a small scale.
- Design the construction of the gasifier for a pilot scale.

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